Numerical simulation of the transport of particles in electrophoretic displays

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Electrophoretic image displays (EPIDs) are a major contestant in the search for electronic paper. Working prototypes have been demonstrated, however, full understanding of the internal physical properties is not achieved yet. In this article, we will present, for the first time, a complete set of formulae that make it possible to simulate the electrical and optical properties of EPIDs. Starting from a theoretical model, that was presented in a previous article, this article gives numerical and graphical results. The set of formulae that was used and their output helps us understand how particles are transported inside a pixel and how this leads to the electrical and optical properties of the display.

Keywords: electrophoretic image display, simulation, electrical, optical.

1. Introduction

1.1. Components of an EPID

The functioning of an electrophoretic image display (EPID) is based on the movement of coloured pigments inside a coloured or transparent liquid. The pigments are added to a solvent together with surfactant molecules to improve stability of the liquid mixture. These surfactant molecules also provide the pigments with a charge. This makes it possible to move the pigment by means of an externally applied electric field. The liquid is placed between two ITO (indium-tin-oxide) coated electrodes. The electrodes are separated by a spacer of typically 100 μm thickness. When a voltage is applied in one direction, the pigments move towards the electrode closest to the observer who sees a pixel with the pigment-colour. When a voltage of the opposite sign is applied, the observer sees a pixel with the liquid colour. In some applications, two kinds of pigments with contrasting colours are used in a transparent solvent. In this case the observed pixel colour is one of the pigment colours based on the applied voltage. By combining these pixels in an array, one can build up a reflective display.

The pigments are neutral molecules with a radius of approximately 0.5 μm. The solvent is a neutral dielectric liquid. Surfactant is added in order to avoid flocculation and precipitation of pigments. When added to the pigments, the neutral surfactant molecules break up into two oppositely charged ions. One ion attaches itself chemically to the pigment, the other ion is attracted due to the Coulomb force.

When this happens to a sufficient number of surfactant-molecules, a charged shell of surfactant-molecules is formed around each pigment which helps avoiding flocculation. This shell is neutralized by a cloud of counter-ions that surrounds it. This cloud is attracted to the pigment due to Coulombic attraction forces from the charged cell. Long ionized surfactant groups can also flock together to form, so-called, micelles. These are small, charged particles that are then present in the pixel in addition to the charged pigments. They have the opposite charge as the pigments. We already proved that these micelles form the major contribution to the electrical current [1]. They are also the source of the generation current, the steady state current that flows through a pixel even when a voltage has been applied for a long time and all charged particles are at rest at the electrodes. Ions are generated in the externally applied field from neutral OLOA molecules and lead to a steady state current.

This system of charged particles becomes even more complex when an external voltage is applied.

1.2. Simulation model

In our theoretical model, we have already described how we will simulate the particle transport and which formulae will be used [2]. We assume the particles to have a normal (Gaussian) distribution. This is close to the real distribution when calculating interparticle forces and gives easy to handle formulae when calculating [3,4]. The voltage dependencies and parameters that we use were already derived from the theoretical model [2]. The average particle distribution is time and voltage dependent in order to model the

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transport of particles due to drift forces like the externally applied electrical field. The standard deviation of the distribution is also time and voltage dependent in order to model the diffusion of particles due to interparticle forces.

We found that there is a great dependence of the electrical and optical response on the voltage that was applied in the previous phase [1]. This voltage defines the starting distribution of the particles and hence has an impact on the response when a new voltage is applied. For reasons of simplicity we will always suppose that this voltage before the simulation or measurement starts has been applied for a sufficiently long time in order to achieve a stable configuration. From now on we will call this previously applied voltage V_1. The voltage applied during the time of simulation or measurement will be called V_2.

In this article we will only give the numerical results. Some parameters differ from the theoretical model, this was sometimes necessary to get a more accurate match between simulation and measurement. The values of all the parameters that are used were obtained by combining the theoretical prediction and optimisation to match the measurements.

We will give results of simulations of how the charged particles move inside a pixel and how this movement leads to the electrical current. We will also investigate how the pigment distribution changes when a voltage is applied and how this leads to the characteristic optical response of an EPID.

2. Particle distribution

2.1. Pigment distribution

The distribution of the pigments is given by

$$n_k(x,t,V_1,V_2) = \frac{N}{\sqrt{2\pi}\sqrt{V_1 v_{op}t}}$$

$$\times \exp - \frac{\left(x - V_2 \left(1 - \frac{1}{\sqrt{1+t+\frac{75}{V_1}}} \right) v_{op}t \right)^2}{2V_1 v_{op}^2 t^2}. \quad (1)$$

The number of pigment particles at a certain distance x from the electrode, at a certain time t after application of the voltage V_2 after long application of a voltage $-V_1$ is given by Eq. (1). This is a Gaussian distribution with a time and voltage dependent average value and standard deviation.

The pigments move along the x-axis from one side of the pixel ($x = 0$) to the opposite side ($x = d$).

This formula is in good accordance with the theoretical predictions [2]. Only the dependence of the average value on V_1 and t was altered in order to take into account that at V_1 = infinity and $t = 0$ the average value is exactly zero.

In order to take into account the presence of the electrode at $x = 0$ and $x = d$ and the fact that these form an impenetrable border for the particles we will add the mirror particles to the total. This is done in the equation

$$n_{pigment}(x,t,V_1,V_2) = n_k(x,t,V_1,V_2) \\ + n_k(-x,t,V_1,V_2) . \quad (2)$$

When the simulation starts, for small values of the time t, hence average particle distribution close to the electrode at $x = 0$, all particles are pressed against the electrode following an exponential distribution [3,4]. This is simulated by adding the mirror particles at $x < 0$ to the ones inside the pixel ($x > 0$).

2.2. Distribution of charge carriers

The distribution of the OLOA micelles is given by

$$n_{charge}(x,t,V_1,V_2) = \frac{1}{\sqrt{2\pi}\sqrt{V_1 v_{\sigma m}t}}$$

$$\times \exp - \frac{\left(x - d + V_2^{0.85} \left(1 - \frac{1}{\sqrt{1+t+\frac{75}{V_1}}} \right) v_{am}t \right)^2}{2V_1 v_{\sigma m}^2 t^2}. \quad (3)$$

The micelles move along the x-axis from one side of the pixel ($x = d$) to the other side ($x = 0$). Since they have the opposite charges of the pigments, they move in the opposite direction when an external voltage is applied.

The same accordance to theory as with the pigments is achieved, with the same remark about the altered dependence of the average particle distribution on V_1. Furthermore was the V_2 dependence of this average value altered slightly. This was necessary in order to have a more accurate match with current measurements. This lower dependence on V_2 (exponent 0.85 instead of 1) can be explained by the fact that the micelles are much smaller than the pigments and have a smaller charge [1], hence the interparticle forces become more important over the drift forces.

2.3. Delay time

We have to incorporate a delay time in the particle movement and distribution. This is necessary because of the field screening of the external field by the charge carriers and image charge effects at the electrodes [1,5].

We will also use a normal distribution for the delay time. The particles leave the electrodes on application of the voltage V_2 with a certain delay time of which the average value and standard deviation are voltage dependent.

The delay time of the OLOA micelles is given by

$$R_{charge}(t_d, V_2, V_1) = \frac{1}{\sqrt{2\pi}\sigma \dfrac{V_1^{0.6}}{V_2^{0.2}}}$$

$$\times \exp\left(-\frac{\left(t_d - T_d \dfrac{V_1^{1.5}}{V_2^{0.15}}\right)^2}{2\sigma \dfrac{V_1^{0.6}}{V_2^{0.2}}}\right). \qquad (4)$$

The values that were used for the average delay time T_d and the standard deviation are $T_d = 0.1$ and $\sigma = 0.5$ for the micelles.

The distribution of the delay time of the pigments is given by

$$R_{pigment}(t_d, V_2, V_1) =$$

$$= \frac{1}{\sqrt{2\pi}\sigma \dfrac{V_1^{0.5}}{V_2^2}} \exp\left(-\frac{\left(t_d - T_d \dfrac{V_1^{1.5}}{V_2^{0.15}}\right)}{2\left(\sigma \dfrac{V_1^{0.5}}{V_2^2}\right)}\right). \qquad (5)$$

With values of $T_d = 75$ and $\sigma = 30$.

The voltage dependence of this delay time had to be altered with respect to the theoretical model. This is not abnormal since the delay time is a more abstract concept which was difficult to derive theoretically from the known formulae.

The delay time of the pigments is less dependent on V_1 and much more on V_2. This is in accordance with what we previously found. They are bigger and more rigid particles, which makes them more susceptible for external drift forces than for interparticle forces. Since this was not considered in the theoretical model, this optimized and matched numerical simulation slightly differs.

The delay time has to be incorporated in the particle distribution in order to become the real, complete distribution. This total distribution of the micelles charge carriers is given by

$$n_{charge,delay}(x, t, V_1, V_2) =$$

$$= \int_0^t n_{charge}(x, t - t_d, V_1, V_2) * R_{charge}(t_d, V_1, V_2)d(t_d) \qquad (6)$$

Figure 1(a) shows n_{charge} in a function of the time at different places inside the pixel $x = 0.2d$, $x = 0.5d$, and $x = 0.8d$. Figure 1(b) shows the same, but for $n_{charge,delay}$.

The applied voltages were $V_1 = 4$ V and $V_2 = 4$ V. The influence of the delay time can be seen clearly. In Fig. 1(a), the peak amount of particles at $x = 0.8d$ passes fast in a narrow band. Remember that the micelles travel from $x = d$ to $x = 0$. At $x = 0.2d$ the peak is reached later and it is also broadened, this is due to the diffusion forces.

When the delay time is incorporated, the peak values are reached later and the distribution is more spread out because of the standard deviation of the delay time.

The incorporation of the delay time is done in the same way for the pigments. The exact calculation is given later together with this of the optical response. Figure 2 shows the pigment distribution between the two electrodes at three different moments ($t = 7$ s, $t = 12$ s, and $t = 17$ s from left to right). We see that the group of pigments moves to the opposite electrode under the influence of drift and spreads out due to diffusion. The applied voltages were $V_1 = -10$ V and $V_2 = 20$ V.

2.4. Summary

We only showed simulation results of particle distributions. These cannot be matched to measurements since it is impossible to look into a display from the side in order to see how the particles are distributed. The parameters used in the simulation were optimised, if necessary, by comparing
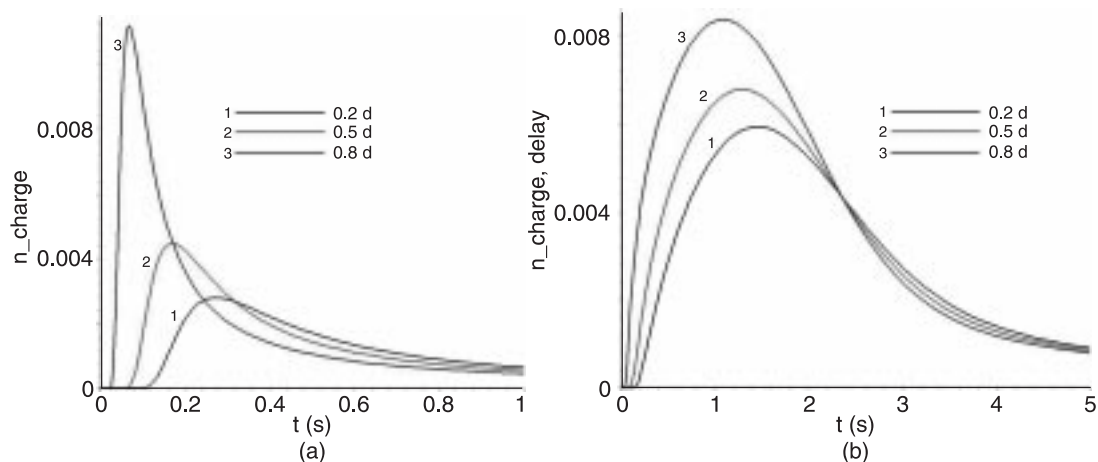

Fig. 1. Variation of the number of charged micelles with time at different positions in the pixel: without counting in the delay time, $x = 0.2d$, $x = 0.5d$ and $x = 0.8d$. The applied voltages were $V_1 = 4$ V and $V_2 = 4$ V (a), with the delay time counted in $x = 0.2d$, $x = 0.5d$ and $x = 0.8d$. The applied voltages were $V_1 = -4$ V and $V_2 = 4$ V (b).
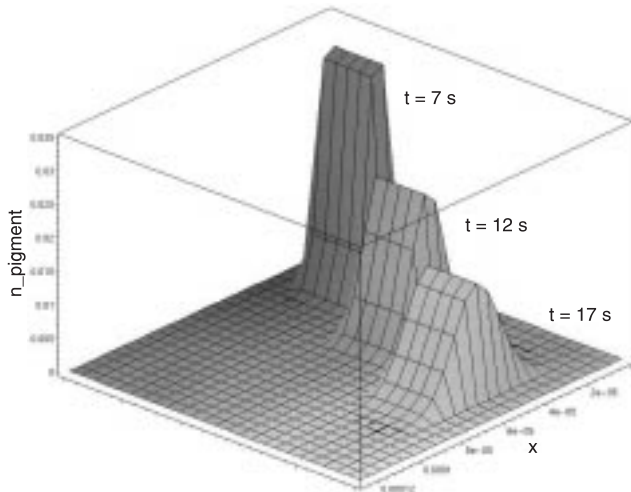
Fig. 2. Variation of the number of pigments along the pixel thickness at different moments in time $t = 7$ s, $t = 12$ s and $t = 17$ s. The applied voltages were $V_1 = -10$ V and $V_2 = 20$ V.

the output of the simulation to electrical and optical measurements. In physical understanding of the display of particles transport and distribution, it is necessary to predict the electrical and optical responses, while simulating the reverse order was used. The understanding of the particle distribution which was mentioned above was actually a consequence of the matching to electrical and optical results. These are shown in the following paragraph.

Our simulation which uses a Gaussian distribution for the charge carriers (micelles) and the pigments is sufficient and is in accordance with what we would expect. The group of particles moves across the pixel under the influence of the drift forces and spreads out due to diffusion. The absolute velocities at which this happens were unknown until they can be deduced from the formulae mentioned above. At any given time it is possible to calculate the pigment and charge distribution inside a pixel. This can be done for any value of the applied voltage V_2 and the previously applied voltage V_1. The voltage V_1 has to be held for a sufficiently long time in order to reach a stable configuration. Through the parameter N, the amount of particles that is present, the influence of pigment and OLOA concentration can be counted in. In the future, we hope to find a connection between the particle velocity and physical properties like mobility, particle radius and charge, and viscosity.

We will not give too much output since these are only the first results and to avoid a too elaborate article.

3. Electrical and optical simulation

3.1. Electrical currents

We already proved that the micelles from the major contribution to the current [1]. This is confirmed by the values of the average and diffusion velocity that are used in the simulation.

The value of the parameters v_{am} and v_{sm} of the charge carriers is 1E-4 m/s and that of the pigments is 2E-7 m/s. We already assumed a connection between the parameters v_{am}, $v_{\sigma m}$, v_{ap}, and $v_{\sigma p}$ the mobility and viscosity [2]. The fact that the drift and diffusion parameters in the simulation are equal (apart from their voltage dependence) is a confirmation of the fact that they are linked to the same constant, physical parameter.

From the values above we see that the pigments move at a velocity that is 500 times slower and therefore have a smaller influence on the current. Remember that this is not the real average and diffusion velocity since we also have to incorporate the delay time and the voltage dependence.

Using the distribution of the charge carriers, it is possible to calculate the electrical transient current. The velocity of the charge carriers inside the pixel at a position x and a time t for the given voltages V_1 and V_2 is given by

$$v_{charge}(x,t,V_1,V_2) = \frac{\dfrac{d(n_{charge}(x,t,V_1,V_2))}{dt}}{\dfrac{d(n_{charge,delay}(x,t,V_1,V_2))}{dx}}. \quad (7)$$

Using the velocity of the micelles and their distribution, we can calculate the electrical current. This is done in the equation

$$I(t,V_1,V_2) =$$
$$= \int_0^d v_{charge}(x,t,V_1,V_2)n_{charge,delay}(x,t,V_1,V_2)dx + I_{ss}, \quad (8)$$

where I_{ss} is the steady state current which occurs due to the generation of charge when micelles ionize in the electric field. In our simulation we used a simple linear voltage dependence with an exponential relaxing growth in time. This is because the generation current depends on the local particle distribution which stabilizes with a time constant of the same order of magnitude as the particle transition time

$$I_{ss} = 70NV_2 v_{ap}\left(1 - \exp\left(-\frac{t}{0.5}\right)\right).$$

Below we will give three simulation results from which can be concluded that our simulation is in good accordance with measurement. We measured the dependence of the transient current curve on V_1 and V_2. Both simulations give a very good fit. Furthermore is the simulation of the current response to a block wave also in agreement with measurements. The match with the optical measurements that is shown in the following paragraph proves that our model is also useful for optical simulations.

Figure 3(a) shows the simulation of the transient current on application of $V_1 = -10$ V and $V_2 = 0.5$ V, $V_2 = 2$ V, and $V_2 = 10$ V. Figure 3(b) shows the measurement of this current. Figure 4(a) shows the simulation of the transient current on application of $V_2 = 2$ V and $V_1 = -2$ V, $V_2 = -5$ V,

and $V_2 = -8$ V. Figure 4(b) shows the measurement of this current. Figure 5(a) shows the simulation of the transient current on application of $V_1 = 1$ V and $V_2 = -1$ V; $V_1 = 2$ V and $V_2 = -2$ V; and $V_1 = 4$ V followed by $V_2 = -4$ V. Figure 5(b) shows the measurement of this current.

From the shape of the curves and their position with respect to each other, it is clear that the model is in accor-

dance with a measurement of the currents and their voltage dependencies. For the constant V_1 and increasing V_2 [Figs. 3(a) and 3(b)] the current peak comes earlier, increases in amplitude and the transient time becomes shorter. For the constant V_2 and increasing V_1 [Figs. 4(a) and 4(b)] the current peak comes later, lowers in amplitude and the transient time becomes bigger. On application of a block wave
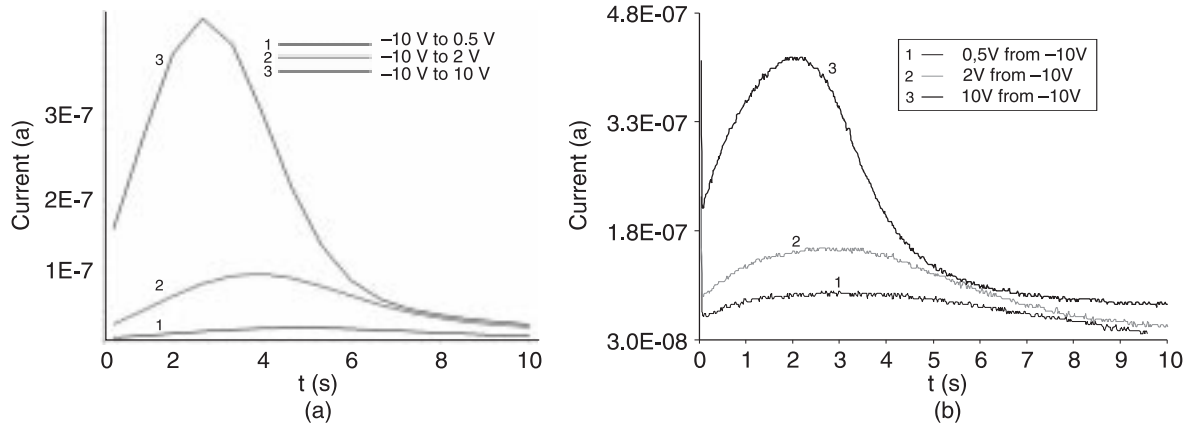

Fig. 3. Simulation of the transient current on application of $V_1 = -10$ V and $V_2 = 0.5$ V, $V_2 = 2$ V, and $V_2 = 10$ V (a). Measurement of the transient current on application of $V_1 = -10$ V and $V_2 = 0.5$ V, $V_2 = 2$ V, and $V_2 = 10$ V (b).
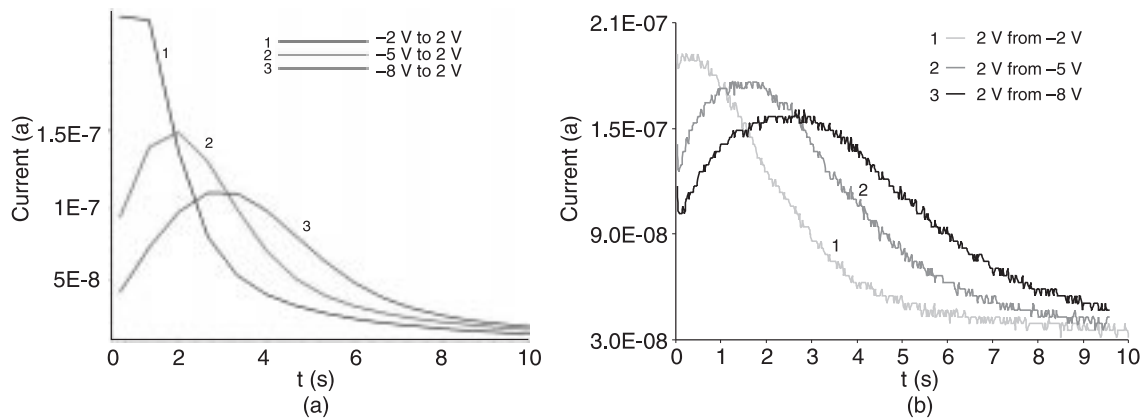

Fig. 4. Simulation of the transient current on application of $V_2 = 2$ V and $V_1 = -2$ V, $V_2 = -5$ V and $V_2 = -8$ V (a). Measurement of the transient current on application of $V_2 = 2$ V and $V_1 = -2$ V, $V_2 = -5$ V and $V_2 = -8$ V (b).
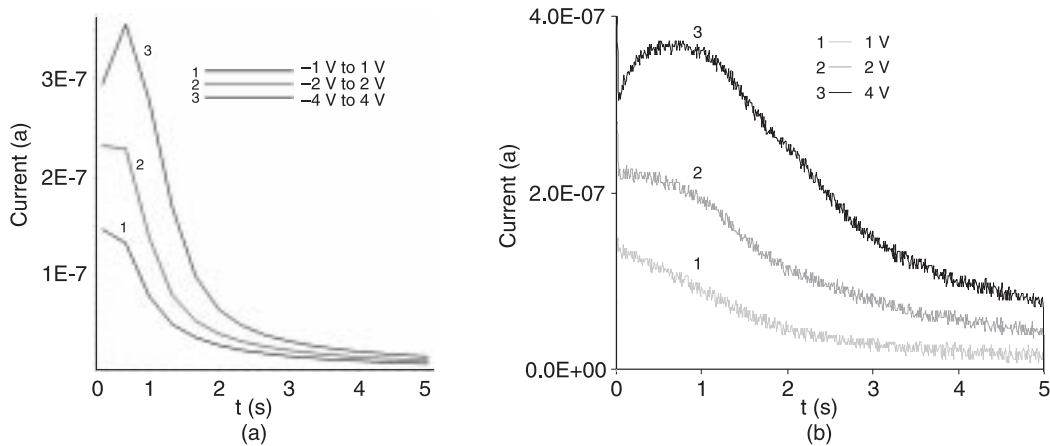

Fig. 5. Simulation of the transient current on application of $V_1 = 1$ V, $V_2 = -1$ V, $V_1 = 2$ V, $V_2 = -2$ V and $V_1 = 4$ V, $V_2 = -4$ V (a). Measurement of the transient current on application of $V_1 = 1$ V, $V_2 = -1$ V; $V_1 = 2$ V, $V_2 = -2$ V; and $V_1 = 4$ V, $V_2 = -4$ V (b).
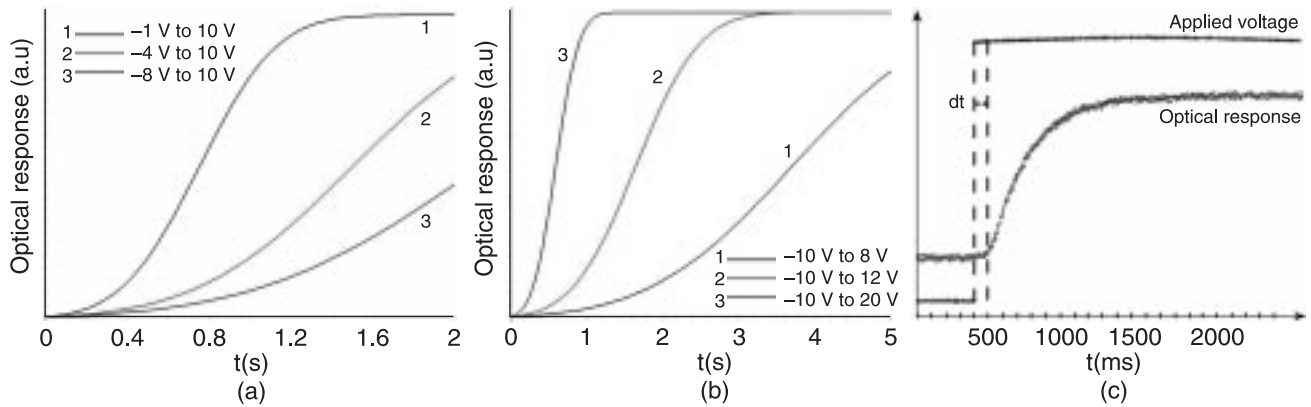
Fig. 6. Simulation of the optical response for: $V_2 = 10$ V and $V_1 = -1$ V, $V_1 = -4$ V and $V_1 = -8$ V (a), $V_1 = -10$ V and $V_2 = 8$ V, $V_2 = 12$ V and $V_2 = 20$ V (b). Measurement of the optical response on application of $V_1 = -20$ V and $V_2 = 20$ V (c).

($V_1 = s_2$) with increasing amplitude, the current peak comes later. For low voltages there is not even a peak. Why this happens was explained in a previous article [1].

3.2. Optical response

The optical response is given by Eq. (9) [5]

$$J(t, V_1, V_2) = \int_0^t R_{pigment}(t_d, V_1, V_2)$$

$$\times \left[\int_0^d n_{pigment}(x, t - t_d, V_2, V_1) e^{\alpha(x-d)} dx \right. \quad (9)$$

$$\left. + \int_d^\infty n_{pigment}(x, t - t_d, V_2, V_1) dx \right] d(t_d)$$

Figure 6(a) shows the simulation of the optical response when $V_2 = 10$ V and $V_1 = -1$ V, $V_1 = -4$ V, and $V_1 = -8$ V. Figure 6(b) shows simulation of the optical response when $V_1 = -10$ V and $V_2 = 8$ V, $V_2 = 12$ V, and $V_2 = 20$ V. Figure 6(c) gives the measurement of the optical response on application of $V_1 = -20$ V ~åç $V_2 = 20$ V.

The shape of the optical response fit the measured value. Since Eq. (9) is a correct equation [5], the pigment particle distribution $n_{pigment}(x, t, V_1, V_2)$ and the pigment delay-time distribution have to be correct in order to become a correct optical response. This is a final double check that proves that our model is applicable and complete to simulate both electrical and optical properties.

4. Conclusions

We presented a complete set of formulae which makes it possible to simulate the transport and distribution of particles inside an EPID. From matching the measured transient current curves and their time and voltage dependence it was possible to optimize the parameters that define the transport of the charged micelles. By comparing the pig-

ment distribution and time and voltage dependence to the distribution of the micelles and by matching to measured optical response curves, it was also possible to simulate the transport of pigments.

By using the formulae, the measured transient current and optical curves at different values of V_1 and V_2 can be simulated.

The actual time and voltage dependent distribution of the particles cannot be inspected by referring to measurements, it is not possible to look inside a pixel from the side and see how the particles are transported. However, the agreement with theoretical predictions is very good and the electrical and optical simulations which use the particle distribution form a double check to decide that the model is applicable.

Acknowledgements

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