One- and two-dimensional finite element analysis of humidity ingress in polymeric materials

Stefan Mitterhofer, Marko Jankovec, Marko Topič
Faculty of Electrical Engineering
University of Ljubljana
stefan.mitterhofer@fe.uni-lj.si, marko.jankovec@fe.uni-lj.si, marko.topic@fe.uni-lj.si

Abstract – Humidity ingress in polymeric materials, used as encapsulants in photovoltaic (PV) modules, is modeled with finite element analysis (FEA). Two different meshes are created according to an experimental setup to analyse humidity ingress in-situ. The first is a rectangle, \((0.001\times0.72)\) mm, describing diffusion only in one dimension. The second describes the two-dimensional cross-section of the humidity sensor and the polymer around it in the experiment. The weak form of the differential equation is obtained from Fick’s laws, describing humidity ingress in materials with a constant diffusion coefficient.

Various parameters of the simulations and their impact on the results are analysed. Diffusion coefficients of the materials are extracted by fitting the simulations to the experimental results. Depending on the different polymers analysed, the two models vary in their success to fit the measurement data, resulting in a high uncertainty for the determination of the diffusion coefficients. Differences are attributed primarily to the limitations of the Fickian diffusion model, which describes an idealized case.

1 INTRODUCTION

Ingress of humidity into photovoltaic (PV) modules is a crucial factor for various degradation modes observed in field installations and operations. They include effects on the polymer itself, for example a reduction of its resistivity to sodium ion ingress, increasing cell-to-frame leakage currents and exacerbating potential induced degradation (PID) [1]. Furthermore, the moisture can corrode the cell metallization [2, 3]. Also the interface between encapsulant and cell, or encapsulant and backsheet, is affected. Humidity has been linked to a reduction of adhesion strength and delamination [4, 5].

The simplest mathematical model describing the diffusion of a substance in a material is Fickian diffusion [6]. Based on the laws formulated by Fick, various attempts have been made to calculate or simulate humidity ingress in polymeric materials [7, 8].

Due to its importance in PV and other fields, the model was expanded in different ways to account for differences in the properties of polymers and penetrants. Factors influencing the ingress include, but are not limited to [9]:

- polymeric structure: degree of crystallinity, thermal and mechanical histories
- penetrant size and nature
- physical conditions, for example temperature \((T)\) and pressure

In the case of PV modules and encapsulants used therein, the experimental verification of these models over a long period using in-situ measurements is lacking in literature.

To measure the humidity ingress in-situ, an experimental setup using miniature T and relative humidity (RH) sensors, Sensirion SHT 25, has been developed [10]. Various polymeric compounds, commonly used as encapsulants in PV modules, have been analysed by encapsulating the sensor strips between two sheets of the polymer [11]. One sensor outside those sheets is used to measure the conditions in the air.

The purpose of this work is to analyse Fickian diffusion and its applicability to simulate humidity ingress into the encapsulants by comparing the simulation results with in-situ measurement data. Two different meshes are used: one approximating the one-dimensional case, and one describing the entire geometry in two dimensions.

In section 2, first the Fickian diffusion model is presented. Then the meshes and the parameters of the simulations are given. In section 3, the results of the simulations are presented, and the impact of the variation of the simulation parameters is analysed. In section 4, both simulations are compared to each other and to the experimental results of different polymers. Diffusion coefficients of the polymers are extracted from the second model.

2 SIMULATION MODEL

2.1 Fickian diffusion

Fick’s laws describe the diffusion [6]. Fick’s First Law (1) describes the rate of transfer of the diffusing substance per unit area \(F\):

\[
\dot{m} = -D \frac{\partial C}{\partial x}
\]
\[ F = -D \frac{\partial C}{\partial x} \quad (1) \]

Here, \( D \) is the diffusion coefficient and \( C \) the concentration of the diffusing substance. \( D \) is generally dependent on the materials and changes with T. Fick’s Second Law (2) describes the diffusion over time:

\[ \frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left( D \cdot \frac{\partial C}{\partial x} \right) \quad (2) \]

In the two-dimensional case, with a constant diffusion coefficient, equation (2) becomes:

\[ \frac{\partial C}{\partial t} = D \cdot \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) \quad (3) \]

2.2 The meshes

Two meshes are used. One-dimensional diffusion is approximated by a rectangle with a width of 0.001 mm, and a length of 0.72 mm according to the experiment. The two-dimensional mesh, shown in figure 1, describes a cross-section across the sensor strip, indicated by the blue line in figure 2 (left). Figure 2 (right) shows a sensor strip encapsulated in a thermoplastic olefin (TPO). The width of the strip is 12 mm. The thickness of the polymer layer is 0.45 mm. However, the sensors have a small indentation, in which the sensing area of the device is located. This window has a depth of 0.3 mm.

![Figure 1: Two-dimensional mesh of the setup (cross-sectional view).](image1)

![Figure 2: Right: Top view of encapsulated sensor strip. Left: Close-up view of a sensor.](image2)

There are two other empty spaces along the cross-section in addition to the sensor’s window: An area between the sensor and a capacitor \( C \), and an area between the capacitor and the printed circuit board (PCB). During lamination, these empty spaces are filled up with the encapsulant, reducing the thickness of the layer directly above. Thus, cosine-shaped indentations at the upper boundary of the mesh are added to the simulation. They reduce the total distance between the boundary to the air, and the sensor area to 0.72 mm.

A polymeric compound is used in the sensor to measure the humidity. This polymeric compound is suspected to have a high solubility, as a result of previous simulations [12]. Thus, it can serve as a water tank in the experiment. This is simulated by moving the barrier behind the sensor’s window, creating a hole filled with more elements in the mesh, shown in figure 2.

In one strip, three sensors are encapsulated, whereas the fourth sensor is exposed to the air.

2.3 Weak form of the differential equation

The software FreeFEM++ is used to solve the differential equation (3). The weak form of the equation is needed as input for the software. Because the expected result is the evolution of the solution over time, the implicit Euler method is used. The time is split into short intervals \( \delta t \). The solution of equation (3) at the time-step \( m \) at a position \( (x,y) \) is denoted \( C^m \).

\[ C^m(x,y) = C(x,y,m \cdot \delta t) \quad (4) \]

With this discretization, the weak form of equation (3) is obtained, which can be solved at each time-step:

\[ \int_{\Omega} \left( \delta t \cdot D \cdot \nabla C^m \cdot \nabla v + C^m v \right) - \int_{\Omega} C^{m-1} v = 0 \quad (5) \]

Here, \( v \) is any function \( v \in H^1(\Omega) \), and \( \Omega \) is the area of the mesh. \( \delta t \) does not have to be the same each step and can vary. In this case, \( m \cdot \delta t \) in equation (4) is exchanged by the sum of the times of all individual time-steps up to step \( m \).

If \( T \) is constant, \( RH \) is linearly dependent on the concentration \( C \). Thus, in the following \( C \) denotes \( RH \) measured by the sensor or simulated.

2.4 Initial and boundary conditions

In the experiment, the sensor strips are put inside a climatic chamber at 20% \( RH \) for a certain amount of time until the entire encapsulant stabilizes. Because the sensors have a certain uncertainty, their initial measurement varies. Thus, one of the measurements of the encapsulated sensors after stabilization is taken as initial condition for \( C \) in the air and in the entire mesh.

After the sensors stabilize, the \( RH \) in the chamber is increased to 40%, 60% or 80%, respectively. A Dirichlet boundary condition is added to the upper boundary of the mesh \( \Gamma \), which is equivalent to the interface between air and polymer.
However, in the experiment, the climatic chamber takes some time to adjust to this new value in its entire volume. Therefore, the boundary takes the measured value of RH in the air at each time-step.

\[ C_\Gamma = C_{\text{air}} \]  

(6)

The other boundaries are simulated as barriers for the diffusion: The PCB, the capacitor and the sensor itself.

3 SIMULATION RESULTS

3.1 One-dimensional case

Two parameters are varied and their influence on the results analysed:

- The diffusion coefficient \( D \)
- The depth of the hole behind the sensor

The results are given as a time evolution of RH at the point in a distance of 0.72 mm from the boundary to the air, in the sensor’s window.

3.1.1 Variation of the diffusion coefficient

Figure 3 shows the simulations with various values for \( D \) in \([10^{-10}, m^2s^{-1}]\). The other parameters, RH in the air at the start \( C_S \) and at the end \( C_E \), and the depth of the hole behind the measuring area of the sensor, are given in table 1.

Humidity ingress is slower for lower values of \( D \), and faster for higher values of \( D \), as expected. But the shape of the curve doesn’t change. It is only translated to an earlier or later stage in time. Outside of deviations in the very early stages of humidity ingress, and the last stages near the saturation value, it has a linear shape.

3.1.2 Variation of the depth of the hole

Changing the depth of the hole behind the sensor is equivalent with a variation in the sensor polymer’s solubility. The simulated RH measured by the sensor in the early stages of water ingress does not exhibit any significant changes, shown in figure 4. However, as time progresses, a larger depth and equivalent a higher solubility of the polymer slow down further ingress. In this case, the polymer acts as a water tank, delaying the saturation of RH in the encapsulant and changing the shape of the humidity ingress curve. The parameters used in this simulation are given in table 2.

3.2 Two-dimensional case

3.2.1 Variation of diffusion coefficient and hole’s depth

Varying diffusion coefficient and hole depth have the same effect as in the 1-dimensional simulations. Figure 5 shows a comparison between the 1-dimensional (dashed) and the 2-dimensional case (straight line). Three different values for \( D \) are shown: \(10^{-11} m^2s^{-1}, 5 \cdot 10^{-11} m^2s^{-1}\) and \(10^{-10} m^2s^{-1}\). The parameters are given in table 1.

Figure 6 shows the same comparison. Three different values of the depth of the hole are shown: no hole, 0.5 mm and 2 mm. The parameters are given in table 2.

Removing the hole affects the initial measurements, when humidity is first noticed by the sensor, only in

Table 1: Parameters used in the simulation analyzing the impact of different values of \( D \).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_S )</td>
<td>20 %</td>
</tr>
<tr>
<td>( C_E )</td>
<td>80 %</td>
</tr>
<tr>
<td>( D )</td>
<td>( 1 \cdot 10^{-10} m^2s^{-1} )</td>
</tr>
<tr>
<td>Depth of hole</td>
<td>varied</td>
</tr>
</tbody>
</table>

Table 2: Parameters used in the simulation analyzing the impact of different depths of the hole.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_S )</td>
<td>20 %</td>
</tr>
<tr>
<td>( C_E )</td>
<td>80 %</td>
</tr>
<tr>
<td>( D )</td>
<td>( 1 \cdot 10^{-10} m^2s^{-1} )</td>
</tr>
<tr>
<td>Depth of hole</td>
<td>varied</td>
</tr>
</tbody>
</table>
the 1-dimensional case. This very early stage is not affected using the 2-dimensional model.

Figure 5: RH at the sensor over time for different values of $D \cdot 10^{-10} m^2 s^{-1}$.

Figure 6: RH at the sensor over time for different values of the depth of the hole [mm].

### 3.2.2 Variation of the encapsulant’s thickness

The thickness of the encapsulant above the sensor is varied. The results are shown in figure 7, the other parameters given in table 3. The thickness is given as the depth of the sensor window (0.3 mm) plus the thickness of the polymer layer above it, which varies.

If the layer is thick, varying it just changes the time needed for the humidity ingress. It does not change the shape of the curve. However, if it is lowered further, close to the usual thickness of a polymer layer used in PV module manufacturing, the shape of the humidity ingress curve begins to change in the late stages of the ingress.

Figure 7: RH at the sensor over time for different values of the encapsulant thickness [mm].

### Table 3: Parameters used in the simulation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_S$</td>
<td>20 %</td>
</tr>
<tr>
<td>$C_E$</td>
<td>80 %</td>
</tr>
<tr>
<td>$D$</td>
<td>$1 \cdot 10^{-10} m^2 s^{-1}$</td>
</tr>
<tr>
<td>Depth of hole</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

### 4 COMPARISON WITH MEASUREMENT DATA

#### 4.1 Parameter optimization

Four different polymers are analysed:

- Ethylene-vinyl acetate (EVA), which is the most commonly used polymer in PV encapsulation [13]
- Thermoplastic olefin (TPO)
- Polyolefin elastomer (POE)
- Ionomer

The simulation parameters, $D$ and hole’s depth, are varied to achieve the best possible fit with the experimental data. However, throughout all experiments, the solubility of the sensor’s polymer does not change. Thus, the depth of the hole is kept constant for the simulations of all polymers after initial optimization. It is optimized with EVA, because this polymer yields the best fit between simulation and experiment. Out of the four encapsulants analysed, it is best described by the Fickian diffusion model. The results of the simulations for EVA are shown in figure 8.

Figure 8: RH at the sensor over time for EVA.

The simulations with the mesh describing the entire geometry of the experiment yield a more accurate fit with the experimental results compared to the simplified mesh. However, there are several differences between simulation and measurement, especially in the later stages of the ingress. The suspected main reasons are:

- Fickian diffusion is an idealized case. $D$ is in general dependent on the concentration.
- The sensors show a certain inaccuracy, especially at high values of $T$ and $RH$, quantified in their datasheet [14]. These
inaccuracies are generally a drift towards higher measured RH values [10].

4.2 Diffusion coefficient

To obtain an error range for the diffusion coefficient, the simulations are optimized at three points, shown at the example of Ionomer in figure 9:
- Initial stage, when the moisture first penetrates through the entire encapsulant layer and is measured by the sensor.
- General ingress, which tries to give the most accurate fit for the entire ingress curve.
- Late stage, when the moisture ingress reaches saturation levels inside the sensor.

Figure 9: Comparison between simulation and experiment for Ionomer with different values of $D$.

There are differences up to 37.5% between the obtained values for $D$ from the one- and two-dimensional model. However, due to the bad fit of the first model, the error range of the results is relatively large, allowing no accurate determination about the diffusion coefficients from it. Thus, only the results of the second model are given in table 4.

Table 4: Results of the optimization of $D$ with the second model.

<table>
<thead>
<tr>
<th>Polymer</th>
<th>$D$ (min)</th>
<th>$D$</th>
<th>$D$ (max)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EVA</td>
<td>1.2</td>
<td>1.5</td>
<td>1.7</td>
</tr>
<tr>
<td>TPO</td>
<td>0.14</td>
<td>0.4</td>
<td>1.5</td>
</tr>
<tr>
<td>POE</td>
<td>0.3</td>
<td>0.8</td>
<td>1.5</td>
</tr>
<tr>
<td>Ionomer</td>
<td>0.026</td>
<td>0.05</td>
<td>0.12</td>
</tr>
</tbody>
</table>

These values point out the relatively good fit of the model with EVA. The worst fit, with the largest discrepancy between experiment and simulation, and the largest error range, is observed with TPO.

5 CONCLUSIONS

The Fickian diffusion model and the meshes for the FEA have been presented. Various simulation results with different parameters have been given. Varying the diffusion coefficient does not change the shape of the moisture ingress curve, but translates the same curve to an earlier or later period.

A hole behind the sensor area in the mesh was used, simulating a polymer used in the sensor. Variations to the hole’s depth show the impact the miniature sensors itself can have on the measurements.

The simulation results were compared to measurement data with different polymers. Diffusion coefficients and their possible error ranges were extracted. The accuracy of the Fickian diffusion model varies for the different polymers. Out of four analysed materials, only one (EVA) shows a good fit between experiment and simulation. These results emphasize the need for further work on the mathematical model, and the differences between the mechanisms of humidity ingress in various polymers.

Acknowledgments

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References


