Validation and Application of a Numerical Code for Energy Performance of Glazing Systems based on Semi-Transparent Organic Photovoltaic Elements

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Abstract

In this paper, the results of the validation modeling of glazing systems and an application based on Semi-transparent organic photovoltaics (ST-OPVs) are reported. A numerical code was developed for research purposes to improve the glazing modeling in building energy performance taking into account spectral radiative properties in glazing, building envelope integrated technologies and energy-saving strategies. The accuracy and the reliability of the presented code were appropriately tested by means of the ANSI/ASHRAE Standard 140/2011 with mean root square error values lower than one degree centigrade compared with the values available in the presented range. Also, it is presented an approach to integrate solar harvesting of solar energy by glazing systems with an application based on ST-OPVs elements, with power generation around 75W in each glazing, equivalent to an efficiency of 9%.

Introduction

One of the most common need in commercial and residential buildings regarding energy is its consumption, that is, they are constantly in need of energy efficiency. In this context, energy simulation in buildings is an essential procedure worldwide, which ultimately saves energy and renders building operations more efficient. At the same time, certification is a mandatory requirement, for example, in the form of the Leadership in Energy and Environmental Design (LEED) certificate created by the U.S. Green Building Council (2018) and the Brazilian Program of Labelling in Buildings PBE-Edifica (2018). Some of the objectives of energy simulation are: the investigation of new efficiency strategies for buildings; assessment of the most suitable design options; compliance with legislation; and economic analyses that determine how impactful conservation is. Negendahl (2015) describes a significant number of simulation tools that have been developed and used to support the design, construction, retrofit, and operation of energy efficiency in buildings. According to Diakaki et al. (2008), the continuous development and the design of next-generation

buildings is important because they promote the integration of renewable energy technologies, including the focus of this study: resources to harvest of solar energy on façades. Solar control glazing with semi-transparent polymer solar cells were investigated by Sun et al. (2018), who identified that the recent progress in the development of polymer solar cells has improved energy conversion efficiency from 3% to almost 9%. Using semiconducting polymers, these solar cells are fabricated from solution-processing techniques and present unique prospects for low-cost solar energy harvesting due to their advantageous materials and manufacture. Li et al. (2012) indicates potential applications of polymer solar cells are broad, ranging from flexible solar modules and semitransparent solar cells in windows to building applications. Buonomano (2016) reports that building energy simulation is still a complicated process that requires modeling and analytical skills for all stages of a project, including development, implementation, and use. The present study is divided into two stages; the validation stage consisted of a comparison according to the ANSI/ASHRAE Standard 140/2011 developed by Judkoff and Neymark (1995), as well as the application of the BESTest methodology and the general criteria and standard procedures available in Testing and Validation of Building Energy Simulation Tool, IEA-SHC (2018). The second stage consisted of the application of the code to evaluate glazing systems based in spectral radiative, multilayer, and internal reflective properties. During this stage, we performed a first approach to evaluate solar energy harvesting by glazing based on semi-transparent organic photovoltaic (STOPV) material. This technology was evidently applicable in a Building-Integrated Photovoltaics (BIPV) area.

Model Description - Physical Approach

In this section, we present the main equations and considerations employed to obtain the variables of the model. The equations were obtained using the principles of transient heat transfer, energy conservation, weather conditions, and thermophysical properties for opaque elements, such as wall, roof, and

floor, and the radiative properties for modeling glazing systems. The approach for the solution of the differential equations is based on the Finite Volume Method (FVM) described by Patankar (1980), and the solution of the system of equations is solved using the Thomas algorithm (TDMA) using a fully implicit scheme. The numerical code was written from scratch using GNU Octave V.3.8.1 for i686-PC-Linux developed by Eaton et al. (2014).

Thermal Zone - Heat Balance

Based on Taylor et al. (1990), the following equation depicts general formulation for multizone modeling:

$$C_z \frac{dT_z}{dt} = \sum_{i=1}^{N_{ci}} Q_{ci} + \sum_{i=1}^{N_{surf}} h_i A_i (T_{si} - T_z) + m_{inf} C_p (T_{\infty} - T_z) + \sum_{i=1}^{N_{zones}} m_i C_p (T_{zi} - T_z) + Q_{sys} \quad (1)$$

where:

$\sum_{i=1}^{N_{ci}} Q_{ci}$ is the sum of the internal loads, $\sum_{i=1}^{N_{surf}} h_i A_i (T_{si} - T_z)$ represents convective heat transfer from the zone surfaces, $m_{inf} C_p (T_{\infty} - T_z)$ is infiltration of outside air, $\sum_{i=1}^{N_{zones}} m_i C_p (T_{zi} - T_z)$ represents interzone air mixing, and Q_{sys} represents the system output. Internal loads occur when interferences such as lighting, electrical equipment, people, among others are present in the zone, and are specified as such in the input. Heat transfer through zone surfaces is computed from the surface convection coefficient h_i and the surface temperature T_{si} , where each surface or surface element (wall, window, roof, etc.) is assumed to be isothermal. The surface temperatures are computed by performing heat balances on the inside and outside surfaces, using FVM to relate conditions across the element. Doors and windows open to the outside environment are sources of infiltration rates are specified as an infiltration volume (V_{inf}) input. To compute the thermal zone temperature, we have employed the ANSI/ASHRAE 140 BESTest methodology as follows:

- There must be only one thermal zone
- Heat or Cooling Systems are not available (Free Float condition)
- There are no internal loads

As previously mentioned, the BESTest methodology is quite direct, thus all the conditions for the FF (Free Float) can be met with the following approach:

$$C_z \frac{dT_z}{dt} = \sum_{i=1}^{N_{surf}} h_i A_i (T_{si} - T_z) + m_{inf} C_p (T_{\infty} - T_z) \quad (2)$$

The thermal capacitance C_z is related to the amount of energy stored in the area. To obtain this parameter, the following formula can be applied:

$$C_z = \rho_{air} V_{zone} C_{p_{air}} \quad (3)$$

To solve Equation 2, we have used an iterative numerical solution based on TDMA algorithm and FVM with a fully implicit approach. Table 1 and Table 2 present a brief summary of thermophysical properties defined by the BESTest methodology. Additionally, Figure 1 shows a scheme of the geometrical model.

Figure 1: ANSI/ASHRAE 140/2011-Case 600/900.

Table 1: Specifications of opaque surfaces.

Surfaces	Thickness (m)	U-value (W/m ² K)
Wall	0.087	0.514
Roof	0.141	0.318
Floor	1.208	0.039

Table 2: Windows properties.

Property	Value
Extinction coeff.	0.0196 (1/mm)
Number of panes	2
Pane thickness	3.175 (mm)
Air-gap thickness	13 (mm)
Index of refraction	1.526
Transmittance one Pane	0.86156
Thermal Conduc. Glass	1.06 (W/mK)
Conductance glass pane	333 (W/m ² K)
Exterior Surf. Coeff.	21.00 (W/m ² K)
Interior Surf. Coeff.	8.29 (W/m ² K)
Density of glass	2500 (kg/m ³)
Specific heat of glass	750 (J/kg K)

Glazing Modeling

We have developed a theoretical background for evaluation of radiative properties for transparent media along with the mathematical approach for multi-glazing systems. In this article, the generic termi-

nology of properties are "radiative" instead of "optical" because these properties are analyzed within the thermal wavelength band and this includes the visible spectrum. However, we have indicated in which spectral band each property is located.

The most simple case is that of a complete window system consisting of multiple elements separated by gas gaps. Common practice dictates that calculation of window system properties should be done wavelength by wavelength at normal incidence, but these properties are equally valid if angle-dependent or polarization-dependent properties are available. A recursive procedure was carried out until the transmittance and reflectance of the entire glazing system was determined. According to Rubin et al. (1998) and to the Standard ISO 9050 (2003), it is common practice to determine the τ_i (transmissivity), r_i^f (frontal reflectivity), r_i^b (back reflectivity) properties of each element in the system as a function of wavelength. Then for two elements i and j the net transmittance $T_{i,j}$, the front reflectance $R_{i,j}^f$ and back reflectance $R_{i,j}^b$ for the subunit are given by:

$$T_{i,j} = \frac{T_{i,j-1}T_j}{1 - R_{j-1,i}^b R_j^f}, \quad (4)$$

$$R_{i,j}^f = R_{i,j-1}^f + \frac{T_{i,j-1}^2 R_j^f}{1 - R_{j-1,i}^b R_j^f}, \quad (5)$$

$$R_{j,i}^b = R_j^b + \frac{T_j^2 R_{j-1,i}^b}{1 - R_{j-1,i}^b R_j^f}. \quad (6)$$

In the aforementioned equations, a single subscript refers to the property of a single glazing element whose properties must be measured. Convention dictates that the first and outermost element is turned toward the Sun. Similarly, for triple glazing, system properties can be calculated starting with double-glazing properties calculated above and the measured properties of the third layer that was added.

The absorption $\tilde{A}_j^f$ of each element as part of the stack can be calculated via transmittance and reflectance values of the surroundings obtained using Eq. (7) in addition to the external absorptance of the isolated elements A_j as follows:

$$\tilde{A}_j^f = \frac{T_{i,j-1}A_j^f}{1 - R_{j-1,i}^b R_{j,n}^f} + \frac{T_{i,j}R_{j+1,n}^b A_j^b}{1 - R_{j,i}^b R_{j+1,n}^f}, \quad (7)$$

where:

$$A_j^f = 1 - T_j - R_j^f \quad \wedge \quad A_j^b = 1 - T_j - R_j^b. \quad (8)$$

The formulation can be applied to any multi-layered glazing system, such as to triple and quadruple-pane glazing. In all cases, one should calculate the absorption in each layer using the T and R values calculated

in the previous steps. The final step should always be to calculate the spectral and/or directional average properties as aforementioned, due to the spectral average of radiative properties. Figure 2 shows a scheme of the multiple reflections approach in a double-pane glazing and Figure 3 presents the variation of radiative properties according to incidence angle for single, double, and triple-pane glazing systems, all clear glass.

Figure 2: Multiple reflections in a two pane glazing (BESTest Case 600/900).

Figure 3: Variation of radiative properties with angle of incidence for Single, Double, and Triple Glazing.

Glazing Systems Definitions

Table 3 and Figure 4 present the specification and a graphical scheme for selected Glazing Systems labeled as: a) Type 1 for a clear 3mm single-pane; b) Type 2 for a clear 3mm double-pane; c) Type 3 for a double-pane with low-e coating on surface 3; d) Type 4 for a triple-pane filled with Argon, and low-e coating on surfaces 2 and 5. Figure 5 shows the spectral transmission for selected glazings. Spectral radiative properties for each type were obtained from LBNL (2017).

Table 3: Specification of Glazings.

Type	Glass/Gap Thickness (mm)	Coating position	Coating	Gas fill
1	3	None	None	None
2	3/12.7/3	None	None	Air
3	3/12.7/3	Surface 3	$\epsilon=0.137$	Air
4	3/12.7/3/12.7/3	Surface 2 Surface 5	$\epsilon=0.033$	Ar

Figure 4: Selected Glazing Systems.

Figure 5: Spectral Transmission for Selected Glazing Systems.

Glazings and films integrations

In this section, we unveil the approach to evaluate the radiative properties of the semi-transparent organic photovoltaic material available in the literature. The idea was to model this material as a reflective film added to the interior surface of a double-pane glazing system. As for radiative properties of glazing systems, such as transmittance, reflectance, and absorptance at different incidence angles, Riquelme et al. (2017) introduced numerical integration for directional averages to calculate the radiative properties due to the incidence of solar angles as a continuous function.

Modeling of thin films

Although many unsolved problems remain, the general features of the optical behavior of thin films are reasonably developed. Heavens (1991) indicates that the progress in the methods of studying the structures of films continues to grow, assisting in the problems of interpretation of optical phenomena in films. Meanwhile, further developments in the field of high-speed computing are doing much to reduce the labor involved in studying the properties of multiple-film systems. We will include a summary of the mathematical treatment for thin films based on Schuster (2017), the most recent study, and the classic approaches of Walton (1983), Heavens (1991), and Born and Wolf (1999). The reflective film will be treated as a thin, smooth coating on one side of the glass pane. Figure 6 shows a schematic representation of

the investigated optical system: a thin film on top of a thick substrate. The boundary on the second side of the substrate is not shown. In general, the medium behind the substrate is identical to medium 1 (air).

Figure 6: Thin Film Interaction.

The mathematical treatment of the optics of a metallic composed film presented by Heavens (1991) and Born and Wolf (1999) is based on the index of refraction of the metal, which is a complex number.

$$\hat{n}_2 = n_2 - ik_2 \quad (i = \sqrt{-1}) \quad (9)$$

where n_2 is the (real) index of refraction and k_2 is the extinction coefficient. Snell's law can be still applied, but it leads to a complex value of $\cos \hat{\theta}_2 = x + iy$. Thus to obtain these values,

$$a = \left[\frac{(n_1 \sin \theta_1 n_2)}{(n_2^2 + k_2^2)} \right]^2 \quad \wedge \quad b = \left[\frac{(n_1 \sin \theta_1 k_2)}{(n_2^2 + k_2^2)} \right]^2 \quad (10)$$

then

$$x = \sqrt{1 - a + b + \frac{\sqrt{(1 - a + b)^2 + 4ab}}{2}} \quad (11)$$

and

$$y = \frac{a k_2}{(x n_2)} \quad (12)$$

The amplitude (not energy) reflectance at the interface between media i and j for the incident radiation from medium i is given by

$$\hat{\rho}_{ij} = \frac{(\hat{p}_i - \hat{p}_j)}{(\hat{p}_i + \hat{p}_j)} \quad (13)$$

where,

$$\hat{p}_i = \cos \hat{\theta}_i \hat{n}_i \quad [TE \text{ polarization}] \quad (14)$$

$$\hat{p}_i = \frac{\hat{n}_i}{\cos \hat{\theta}_i} \quad [TM \text{ polarization}]. \quad (15)$$

The amplitude transmittance at an interface is given by

$$\hat{\tau}_{ij} = \frac{2 \hat{p}_i}{(\hat{p}_i + \hat{p}_j)} \quad (16)$$

Note that $\hat{p}_{ji} = -\hat{p}_{ij}$ and $\hat{\tau}_{ij} = 1 - \hat{\rho}_{ji}^2$.

Amplitude transmittance ($\hat{\tau}_f$) within the metallic film is based on its phase thickness and is defined as

$$\hat{d} = \frac{2 \pi d \hat{n}_2 \cos \hat{\theta}_2}{\lambda} \quad (17)$$

where d is the thickness of the film, and λ is wavelength spectra. So that

$$\hat{\tau}_f = e^{-i\hat{d}} \quad (18)$$

When multiple reflections within the film are considered, we are led to expressions for the total amplitude reflectance and transmittance. For radiation incident from medium 1, the expressions are

$$\hat{\rho}_{13} = \frac{\hat{\rho}_{12} + \hat{\rho}_{23} \hat{\tau}_f}{1 + \hat{\rho}_{12} \hat{\rho}_{23} \hat{\tau}_f^2} \wedge \hat{\tau}_{13} = \frac{\hat{\tau}_{12} + \hat{\tau}_{23} \hat{\tau}_f}{1 + \hat{\rho}_{12} \hat{\rho}_{23} \hat{\tau}_f^2}. \quad (19)$$

By reversing the subscripts for radiation incident from medium 3, the energy reflectance and transmittance are given by

$$\rho_{13} = \hat{\rho}_{13} \bar{\rho}_{13} \wedge \tau_{13} = \frac{\hat{\tau}_{13} \bar{\tau}_{13} \hat{\rho}_3}{\hat{\rho}_1} \quad (20)$$

where $\bar{\rho}$ and $\bar{\tau}$ are the complex conjugates of $\hat{\rho}$ and $\hat{\tau}$. Energy is absorbed in the film ($\rho_{13} + \tau_{13} < 1$).

Most of the expressions above are complex. Rather than expanding them to get solutions in terms of real numbers, it is easier to let the computer evaluate the expressions by complex arithmetic. The optical constants, such as refraction coefficient and extinction coefficient, are not available directly at the source, but an estimate of this values can be obtained from the available spectral transmittance. Gao et al. (2017) states that a typical reflectance for a TiO₂ surface, due to the near-infrared reflectance of this composite pigment, is as high as 0.68. Average spectral values were calculated using the Kramer-Konig relations for connecting the real and imaginary parts of any complex function as was presented by Rubin (1985).

Glazing-integrated photovoltaic components

Clarke (2015) describes an approach for an integrated photovoltaic façade based on Buresch (1983), taking into account the façade's temperature in the modeling. Current studies employ this approach to of the ST-OPVs integration in glazings for solar energy harvesting. Solar radiation is transmitted to the surface

of the photovoltaic layer through the cover by the processes described in the following section. Before this flux is applied to the corresponding FV conservation equation, the flux magnitude is reduced to reflect the fact that not all absorbed solar radiation α_i will be converted to heat, since a proportion is converted to electrical energy:

$$\alpha'_i = \alpha_i + q_{ei} \quad (21)$$

where α'_i is the actual absorption and q_{ei} is the PV power output (W), which may be determined from the model:

$$q_{ei} = nc \left[V_i I_g \left(1 - e^{\frac{V_i}{\theta_i \lambda \sigma_i}} \right) - \frac{V_i I_{sc} \alpha'_i}{\alpha'_{i(ref)}} \right]. \quad (22)$$

where θ_i is the temperature (K) of the PV material determined from the heat flow calculation scheme, as well as the first node in the glazing numerical algorithm, V_i the node voltage, I_g the generated current, I_{sc} the short circuit current, λ the electron charge (1.6×10^{19} Coulombs), n the number of series connected cells, c the number of parallel connected cells, and σ the Stefan-Boltzmann constant ($5.67 \times 10^{-8} \text{ W m}^{-2}\text{K}^{-4}$). The generated current is calculated as a function of the solar energy absorbed in the PV layer, α_i when referenced to the solar absorption, $\alpha'_{i(ref)}$, corresponding to the standard test condition.

Characterization of ST-OPV

To characterize the Semi-Transparent Organic Photovoltaic (ST-OPV) material, we will define the photovoltaic properties to model solar harvesting and also radiative properties to evaluate the temperature behavior inside the analyzed thermal zone. To evaluate the photovoltaic power, other data are needed, such as the current and voltage produced by the ST-OPV device at each time step., These values are estimated based on solar irradiation on glazings available via weather files. With the information from Table 5 and based on Sun et al. (2018), Figure 8 was constructed using the single diode PV cell equivalent circuit developed by Bellia et al. (2014), Bayrakci et al. (2014), Altas and Sharaf (2007), and classical Duffie and Beckman (2013). Moreover, the large dots indicate in detail the maximum power point for each silver substrate specimen labelled Ag 10 nm to Ag 20 nm. Table 4 presents the results for the spectral average transmittance values calculated by numerical integration for visible and total available spectrum in Figure 7.

Verification Results for ANSI/ASHRAE Standard 140-2011

This section includes the results of the verification stage. Main data are displayed as graphical figures containing the main variables and their comparison

Figure 7: Transmittance - OPVs.

Table 4: Spectral Average Transmittance for ST-OPVs with Various Electrode Thicknesses.

Class	Visible	Total Spectrum
Ag 10	33.60	27.13
Ag 12	30.53	24.62
Ag 14	28.85	22.40
Ag 16	23.67	19.69
Ag 20	19.49	15.73

Figure 8: Current Density (mA/cm²).

Table 5: Photovoltaic Parameters of Organic Cells with Various Ag Thicknesses under Optimized Conditions.

Class	Efficiency %	V _{oc} V	J _{sc} mA/cm²	FF %
Ag 10	6.8	0.81	12.6	65
Ag 12	7.4	0.81	13.5	66
Ag 14	7.9	0.81	14.4	66
Ag 16	8.4	0.81	15.4	66
Ag 20	9.0	0.81	16.3	67

with available data. Figure 9 presents the results for the comparison of the thermal zone temperature obtained by the numerical code developed and the available range results in the ANSI/ASHRAE Standard 140-2011. We draw attention the alignment of the results for a Clear Cold Day with the range for the two available Cases (600FF Low-mass and 900F Heavy-mass). The same figure allows us to observe the correct modeling by the numerical results referenced at the different thermophysical properties for each base case with a Root Mean Square Error value

lower than one degree centigrade compared with the values available in presented range.

Figure 9: Standard 140-2011 Hourly Free Float Temperatures - Clear Cold day - Cases 600FF and 900FF.

Furthermore, Figure 10 shows the behavior of the thermal zone temperature according to the selected 4 types of glazing systems previously defined in Table 3. These results are based on the modeling of the radiative properties for each glazing type included in the Glazing modeling section, where **Type 1** is a single-pane glazing and **Type 4** is a triple-pane glazing with low-e coating on two surfaces. After this first stage, we were able to validate the numerical code for the evaluation of Glazing Systems, and withal, propose an approach to evaluate the photovoltaic potential in glazings.

Figure 10: Comparison of thermal zone temperature according selected Glazing Systems - BESTest Case Base 600FF.

Results

This section shows the results obtained when modeling a single thermal zone and glazing systems considering the spectral radiative properties, multireflections and an approach for integrating a Semitransparent Photovoltaic material for solar energy harvesting in glazings. First, the results for the thermal zone simulation will contain a comparison between the thermal zone temperature obtained in the BESTest as a reference with the temperatures profiles obtained due to the five different thickness of silver substrate originally labeled as Ag10 to Ag20, as per

Sun et al. (2018). Finally, we will include the results for solar energy harvesting using photovoltaic integration based on Clarke (2015), as previously stated.

Thermal Zone Temperature Results due ST-OPV integration

Figure 11 shows the results for the thermal zone temperature according to the 5 selected ST-OPVs configurations. For this example, we selected the Case Base 900FF and a single-pane glazing with the integrated ST-OPV as a thin film over the external surface of the glazing with the internal pane as substrate following the mathematical approach in the **Modeling of thin films** section.

Figure 11: Thermal Zone Temperature for selected ST-OPVs configuration due Base Case 900FF.

Photovoltaic Modeling Results

This section presents the results in Figure 12. We have taken the same approach as Clarke (2015) in Equation 22 due to the fact that estimated power could be generated by the OPVs integrated to the glazing system. The maximum power generation on presented range is around 78W in each glazing to the January 11th, equivalent to an efficiency of 9%. We would like to point out that the solar energy harvesting behavior follows the available solar data from weather files mainly because the values of generated current (I_g) and node voltage (V_i) produced by the device are estimated based on the solar irradiation available on glazing towards the south at each time step. The importance of the temperature in this model is not so clear because this value is inserted in the decay exponential function and it is likely that this variable influences the performance of the photovoltaic element. However, according to this model, temperature does not have a relevant role. We suggest that future studies evaluate the importance of the temperature due to these types of cells.

Conclusion

The energy modeling for glazing systems is not a simple task, but by directly relating the radiative behavior of glazings to energy modeling, we were able

Figure 12: Estimate Power generation by OPVs based Glazing System.

to obtain a physically consistent model. This study sought to develop a numerical methodological code based on ANSI/ASHRAE Standard 140-2011 Case 600/900 to evaluate the thermal behavior of a single thermal zone due to different glazings. As previously stated, the different glazings were modeled taking into account multiple internal reflections and the spectral radiative properties for each case. This allowed us to evaluate any data on glazing or transparent material as radiative properties (transmittance, reflectance, and absorption) and the so-called "optical constants" as refractive and extinction coefficients. The numerical code was verified in the first stage, where the results for thermal zone temperature are in good agreement with the available "BESTest results range". We conclude that the case 600/900 of the denominated BESTest is an excellent model to evaluate glazing systems because solar energy directly influences the energy behavior in the thermal zone. If the radiative treatment of the translucent element is consistent, the thermal behavior varies and it allows to quantify the energy efficiency due to different configurations of glazing systems. As for the second stage, we presented an approach to evaluate the integration of a photovoltaic element on glazings modeled as a thin film taking into account spectral radiative properties following a detailed mathematical approach. This study contributes to the improvement of energy modeling for future thermal load evaluations of cooling and heating due to solar energy gains during the hot and cold seasons.

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