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ScienceDirect

Solar Energy 81 (2007) 969–976

SOLAR ENERGY

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A single-thin-film model for the angle dependent optical properties of coated glazings

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Received 20 October 2005; received in revised form 1 December 2006; accepted 12 December 2006
Available online 17 January 2007

Communicated by: Associate Editor Darren M. Bagnall

Abstract

Technology for the manufacture of coated glazings with spectrally selective optical properties, such as low-e and solar-control glazings, has been developed in the last few decades. This is leading researchers to develop new optical and thermal models in order to ascertain glazing performance. These new models must accurately reproduce the optical properties for any incident solar angle by using the available experimental data, which often means only information for normal incident radiation. In this paper, a new model is presented that characterizes the angular dependence of coated glazings. To provide a simple, intuitive understanding, this model uses only one thin film to characterize optical performance. In addition an optimization algorithm has been developed to obtain the spectral optical properties of that equivalent film using spectral experimental data under normal incidence. Finally, the model is validated with experimental data and the results are compared with other known models.

Keywords: Thin films; Coated glazing; Optical properties

1. Introduction

During the last few years, new models that reproduce the optical and thermal glazing performance of layers have been developed. These developments have been driven by the need to optimise the energy performance of buildings where heating and air conditioning facilities exist, as well as by the technological progress in the manufacturing of new glazing products with selective spectral properties. These facts have allowed designers, engineers and architects to estimate the effect that new high performance glazings can have on energy consumption and natural lighting (Karlsson and Roos, 2000).

In 1999, a review of several different methods and models was presented, as well as their advantages and disadvantages, resulting in an excellent classification that is still widely accepted (Rubin et al., 1999). In this review, the models are divided into detailed and simplified models. The latter are classified as empirical, semi-empirical, monolithic and thin-film models and monolithic models have been the most widely used. A referenced thin-film model, which uses only a metallic thin film, is described in this paper. In addition to this, an improved optimisation process and a more extensive experimental validation have been included in this presentation.

Some alternative models were also evaluated and validated in the frame of the ADOPT project (Angular dependent optical properties of coated glass and glazing products – Measurement procedures and validation of associated predictive methods), an European Research Project

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doi:10.1016/j.solener.2006.12.002

sponsored within the 4th Framework Programme (Hutchins et al., 2001). Experimental data were obtained by using optical spectroscopy, ellipsometry, X-ray and neutron reflectometry from several sets of coated glazing products (commercial and non-commercial samples).

In this project, one of the most interesting validated models was the semi-empirical model (Roos et al., 2000; and Karlsson and Roos, 2000). This one is simple to implement and assumes that all angle-dependent transmittance decreases from 1 to 0 as a function of the form $y = 1 - x^n$ when x changes from 0° to 90°. It is based on the fact that the angular dependence of the optical properties depends on the category of materials used in the coating. Thus, once the coating type is known, the best curve fit (n value) for the angular solar factor can be obtained and the direct solar transmittance and the total solar energy transmittance for multiple glazings for uncoated or coated glass panes can be calculated. However, the reflectivity of the coated glazing is also needed in order to characterise the thermal performance in multiple glazings.

Moreover, within the group of models simplified by using an equivalent thin-film characterisation model, the hybrid equivalent model algorithm (Montecchi et al., 2001) seems to work very well for the majority of samples used during the validation process of the ADOPT project. As the model used in this paper, the hybrid equivalent model does not need information about the material of the coating although its implementation in computers is more complex.

2. The single-thin-film model

In this paper, the model replaces any complex coating with one single metallic thin film, therefore, it is necessary to find the properties of this thin film that exactly reproduce the optical behaviour of the coating that is being replaced. These properties are the refraction index (n), the extinction coefficient (k), as well as its thickness (d). The main difficulty and the main interest of this method lies in the search procedure for these parameters.

First at all, the equations that control the optical behaviour of a coated glazing composed by several thin films will be described. Secondly, the optimisation process developed in order to obtain the optical properties for the equivalent film will be analysed as well as the method to assure the convergence of the optimisation process. Finally, the results obtained are presented.

The equations that reproduce the optical behaviour of a coated glazing when all optical properties are known are presented.

The scheme of the physical model used in this paper is shown in Fig. 1. A set of thin films can be seen on a substrate of the thickness L. Interface effects in the film and multiple reflections in the substrate influence the values of reflectance (R) and transmittance (T).

R and T for a substrate with a set of films on its coated side can be obtained by using the Ray-tracing method.

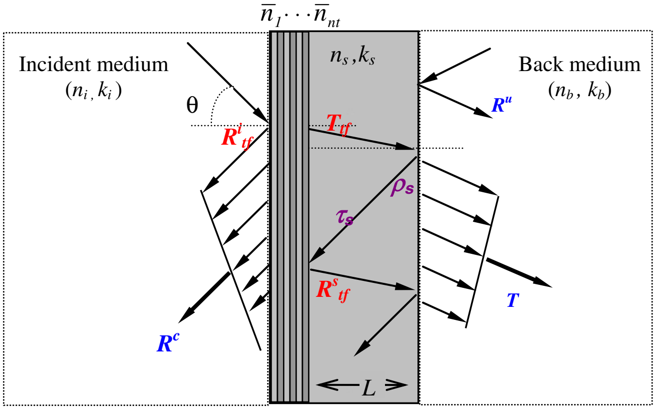

Fig. 1. Single-thin-film model.

$$R^{\mathrm{c}} = R^{i}_{\mathrm{tf}} + \frac{T^2_{\mathrm{tf}}\tau^2_{\mathrm{s}}\rho_{\mathrm{s}}}{1 - R^{\mathrm{s}}_{\mathrm{tf}}\tau^2_{\mathrm{s}}\rho_{\mathrm{s}}} \tag{1}$$

$$R^{\mathrm{u}} = \rho_{\mathrm{s}} + \frac{(1-\rho_{\mathrm{s}})^2\tau^2_{\mathrm{s}}R^{\mathrm{s}}_{\mathrm{tf}}}{1 - R^{\mathrm{s}}_{\mathrm{tf}}\tau^2_{\mathrm{s}}\rho_{\mathrm{s}}} \tag{2}$$

$$T = \frac{T_{\mathrm{tf}}\tau_{\mathrm{s}}(1-\rho_{\mathrm{s}})}{1 - R^{\mathrm{s}}_{\mathrm{tf}}\tau^2_{\mathrm{s}}\rho_{\mathrm{s}}} \tag{3}$$

where ρ_{s} is the reflection coefficient between the substrate and the uncoated side medium, τ_{s} is the substrate transmission coefficient: $\exp(-4\pi k_{\mathrm{s}}L/\lambda)$, where k_{s} is the extinction coefficient of the substrate, and L the thickness of the substrate, $R^{\mathrm{i}}_{\mathrm{tf}}$ is the reflectance from incident medium of the set of the thin films, $R^{\mathrm{s}}_{\mathrm{tf}}$ is the reflectance from substrate medium of the set of the thin films, T_{tf} is the transmission of the set of thin films, R^{c} is the reflectance from coated side of the glazing, R^{u} is the reflectance from uncoated side of the glazing, and T is the transmission of the glazing.

$R^{\mathrm{i}}_{\mathrm{tf}}$, $R^{\mathrm{s}}_{\mathrm{tf}}$ and T_{tf} are obtained considering the interference phenomena between the reflected waves as well as between the transmitted waves, which are generated when the thickness of the film is similar to the incident wavelength.

From the implementation point of view, suitable expressions to formulate these phenomena are obtained by writing the relations between the electric vectors of every thin layer as a function of the Fresnel coefficients. This problem was solved by Abeles (1950) and applied by Heavens (1960):

$$R^{\mathrm{i}}_{\mathrm{tf}} = \left(\frac{a\bar{n}'_i + b\bar{n}'_i\bar{n}'_s - c - d\bar{n}'_s}{a\bar{n}'_i + b\bar{n}'_i\bar{n}'_i + c + d\bar{n}'_s}\right)^2 \tag{4}$$

$$R^{\mathrm{s}}_{\mathrm{tf}} = \left(\frac{a\bar{n}'_s + b\bar{n}'_s\bar{n}'_i - c - d\bar{n}'_i}{a\bar{n}'_s + b\bar{n}'_s\bar{n}'_i + c + d\bar{n}'_i}\right)^2 \tag{5}$$

$$T_{\mathrm{tf}} = \frac{\bar{n}'_s}{\bar{n}'_i}\left(\frac{2\bar{n}'_i}{a\bar{n}'_i + b\bar{n}'_i\bar{n}'_s + c + d\bar{n}'_s}\right)^2 \tag{6}$$

where

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \prod_{j=1}^{nt} \begin{bmatrix} \cos\gamma_j & \frac{\mathrm{i}\sin\gamma_j}{\bar{n}'} \\ \mathrm{i}\bar{n}'\sin\gamma_j & \cos\gamma_j \end{bmatrix}$$

being

$$\bar{n}'_j = \begin{cases} \frac{\bar{n}_j}{\cos\theta_j} & \text{parallel polarization} \\ \bar{n}_j \cos\theta_j & \text{perpendicular polarization} \end{cases},$$

$$\gamma_j = \frac{2\pi \bar{n}_j d_j}{\lambda}, \quad \bar{n}_j = n_j + ik_j,$$

$$\theta_j = \arcsin\left(\frac{\bar{n}_{j-1}\sin\theta_{j-1}}{\bar{n}_j}\right),$$

n_i is the incident medium refraction index, n_s is the substrate refraction index, n_j, k_j are the refraction index and extinction coefficient of the j layer of the coating, d_j is the thickness of the film j.

The reflectivity of both sides can be different. When radiation comes from the uncoated side, reflectivity is obtained by interchanging n_i and n_j indexes.

Transmissivity from both incident sides is equal (Abelès, 1971).

In this paper, the model performance uses only a single thin film. Thus, the number of independent variables from the optimisation process is not very high. The characterisation process described in the following section is used to find the properties of this film.

3. The characterisation process

The characterisation process is a numerical optimisation process in which the optical properties, the extinction coefficient and the refraction index of the thin film for any wavelength are obtained together with the thickness of the thin film. During that process, a system of highly non-linear equations must be solved. This system is obtained by assuming that the optical properties for any wavelength, $R^{\mathrm{i}}_{\mathrm{tf}}$, $R^{\mathrm{s}}_{\mathrm{tf}}$ and T_{tf}, in Eqs. (1)–(3) are known from experimental measurements. The right-hand sides of this set of equations are then calculated by using Eqs. (4)–(6) and by setting estimated values of the thickness, the extinction coefficient and the refraction index of the thin film. The aim of the optimisation process is to find those values which minimise the error between the calculated and experimental optical properties.

This process needs two different sets of experimental data (see Fig. 2). The first one (named set number 1, *set 1*), is formed by the experimental measurements of the whole glazing, substrate and coatings, specifically, transmissivity and reflectivity for any wavelength: $T(\theta = 0°, \lambda)$, $R^{\mathrm{c}}(\theta = 0°, \lambda)$ and R^{u} $(\theta = 0°, \lambda)$. The second set of data (named set number 2, *set 2*) includes the transmissivity and reflectivity of the substrate without the coating ($T_{\mathrm{s}}(\theta = 0°, \lambda)$, $R_{\mathrm{s}}(\theta = 0°, \lambda)$), and the thickness of the substrate. These sets of data are generally available from the manufactures or the international glazing data base maintained by the Lawrence Berkeley National Laboratory in USA Windows (2005) and by WINDAT project (Windat, 2004) in Europe.

The interface reflectivity, ρ_{s}, and the transmission coefficient of the substrate, τ_{s}, can be easily obtained from the experimental data for a substrate under normal incident radiation (*set 2*), and using the standard CEN EN-410. Then, an expression for the properties of the thin film follows from the rearrangement of Eqs. (1)–(3) as a function of the experimental data for the whole glazing (*set 1*), and ρ_{s} and τ_{s}, which are obtained previously

$$R^{\mathrm{s}}_{\mathrm{tf}} = \frac{R^{\mathrm{u}} - \rho_{\mathrm{s}}}{(1-\rho_{\mathrm{s}})^2\tau_{\mathrm{s}}^2 - \rho_{\mathrm{s}}^2\tau_{\mathrm{s}}^2 + \rho_{\mathrm{s}}R^{\mathrm{u}}\tau_{\mathrm{s}}^2} \tag{7}$$

$$T_{\mathrm{tf}} = \frac{T - \rho_{\mathrm{s}}TR^{\mathrm{s}}_{\mathrm{tf}}\tau_{\mathrm{s}}^2}{(1-\rho_{\mathrm{s}})\tau_{\mathrm{s}}} \tag{8}$$

$$R^{i}_{\mathrm{tf}} = \frac{R^{\mathrm{c}} - \rho_{\mathrm{s}}R^{\mathrm{c}}R^{\mathrm{s}}_{\mathrm{tf}}\tau_{\mathrm{s}}^2 - \rho_{\mathrm{s}}T^2_{\mathrm{tf}}\tau_{\mathrm{s}}^2}{1 - \rho_{\mathrm{s}}R^{\mathrm{s}}_{\mathrm{tf}}\tau_{\mathrm{s}}^2} \tag{9}$$

Furthermore, through Eqs. (7)–(9) these properties can be obtained exactly for a set of given values of n, k and d. By making these properties equal to those obtained from

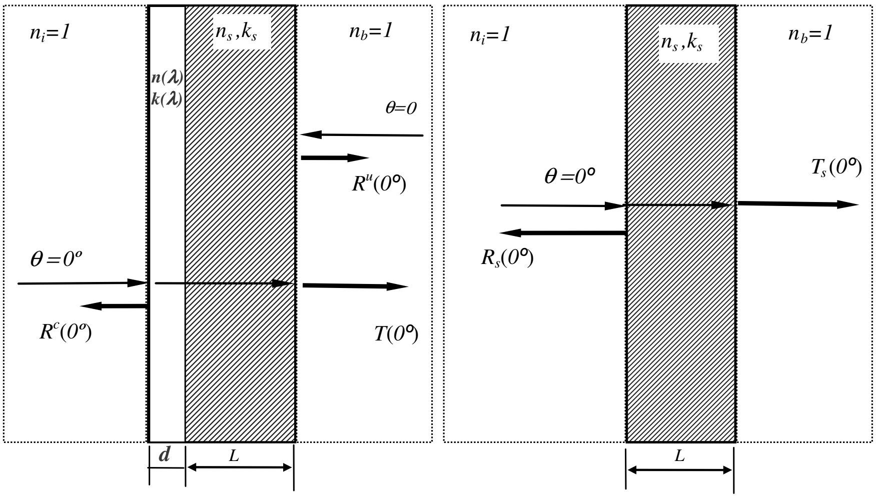

Fig. 2. Sets of experimental data needed for the numerical optimization.

Eqs. (4)–(6), a system of non-linear equations can be solved where n, k and d are the unknown parameters.

An alternative method to solve the system (see Fig. 3) is to seek the set that minimise an objective function. This function represents the accumulative error from the three optical properties of the coating obtained from both ways mentioned before:

$$f_1 = (T_{\mathrm{tf}} - \overline{T}_{\mathrm{tf}}) + (R^{\mathrm{c}}_{\mathrm{tf}} - \overline{R}^{\mathrm{c}}_{\mathrm{tf}}) + (R^{\mathrm{u}}_{\mathrm{tf}} - \overline{R}^{\mathrm{u}}_{\mathrm{tf}}) \tag{10}$$

where the properties are calculated using Eqs. (7)–(9).

Moreover, an optimisation algorithm, in which the minimum of a multivariable, unconstrained, nonlinear function is found (Powell, 1970) has been used to solve the minimisation problem. By using this method, the results for the thickness and the optical properties of the coating make the objective function less than 0.1% in all cases and for any wavelength. This means that the accumulative error of both the transmissivity and the reflectivity is less than 0.1%.

With this method, a different thickness of the coating is obtained for each wavelength, which has no physical meaning. Therefore, the method has been modified by setting the thickness to a fixed value. Finally, an analysis of the influence of the thickness value on the variables of interest was carried out.

From the point of view of the building energy consumption, the variables of interest are the transmissivity and reflectivity of the whole glazing instead of the properties of the coating alone. Therefore, the objective function is changed in order to minimise these other variables:

$$f_2 = (T - \overline{T}) + (R^{\mathrm{c}} - \overline{R}^{\mathrm{c}}) + (R^{\mathrm{u}} - \overline{R}^{\mathrm{u}}) \tag{11}$$

In Fig. 4, a typical shape of the objective function for thin film characterisation is shown. This function shows numerous relative minima that could be adopted as a solution since the accumulative error is less than 0.4%.

Considering any of these minima as a solution, the performance of the glazing for normal incident radiation, that is, for the same incident angle as used in experimental measurements, is quite good. Nevertheless, the analysis of the objective function before the selection of the most suitable minimum is interesting. On the one hand, if the selected values for the refraction index and extinction coefficient are close to the actual values, the glazing performance for oblique angles will be more adequate. On the other hand, the analysis of the objective function will accelerate the optimisation process. And the most important, it will guarantee a solution for any wavelength.

This last point is of special interest when the optimisation process is going to be implemented in software in which the direct participation of the user in the process is

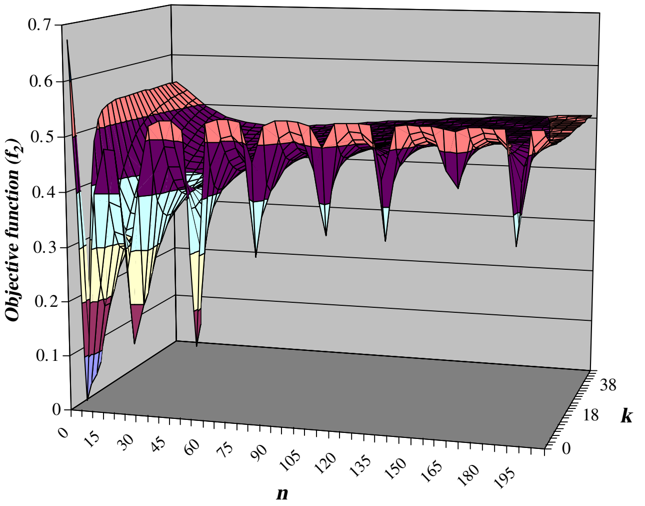

Fig. 4. An example of objective function (Reflectasol Claro®, film thickness: 20 nm).

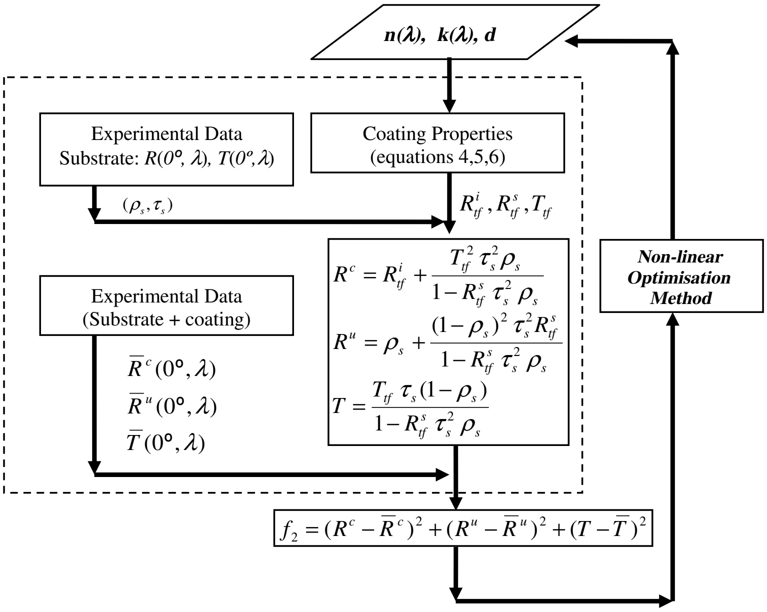

Fig. 3. Numerical optimization schemes to solve the optical properties of coatings.

avoided and the input of the experimental data is the only requirement.

4. Proposed method

The method has been developed in order to guarantee a minimum when the characterisation process is automatic, namely when the user knows nothing about the process. This method is based on the fact that the number of relative minima decreases if the optical thickness (*n d*) of the thin film is fixed to a very small value for any wavelength.

Fig. 5 shows cross-sections of the objective function, which has minima for different values of the thin-film thickness. As can be seen, these curves present only one minimum when the thickness is fixed to 1 nm, which means that the convergence process is guaranteed.

The proposed method assumes that the coating of the glazing is made by only one absorbing thin film. It sets the thickness of this thin film to 1 nm. This very small value for the optical thickness for each wavelength of the solar radiation allows a fast convergence in the optimisation process.

As explained earlier, the selected minimum does not significantly affect the calculated transmissivity and reflectivity under normal incident radiation. However, a selection process that uses a pure functional criterion needs experimental

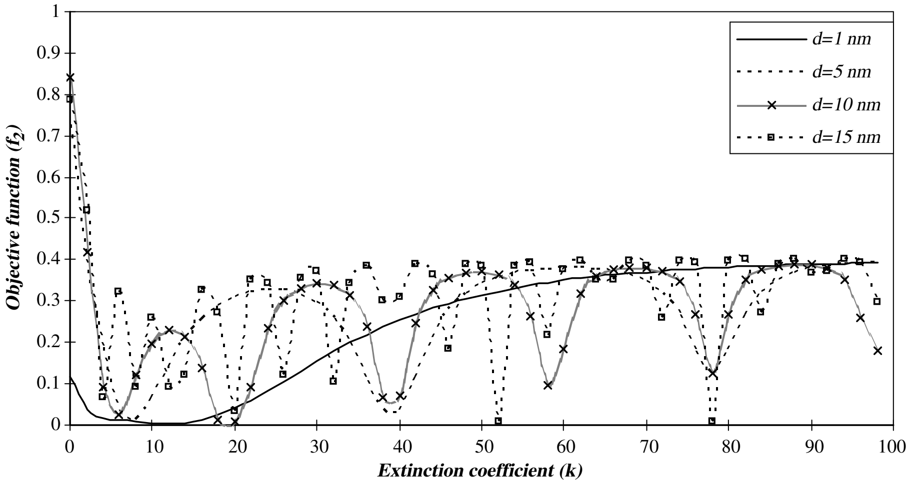

Fig. 5. Cross-sections of the objective function (Reflectasol Claro®, wavelength: 390 nm, fixed refraction index).

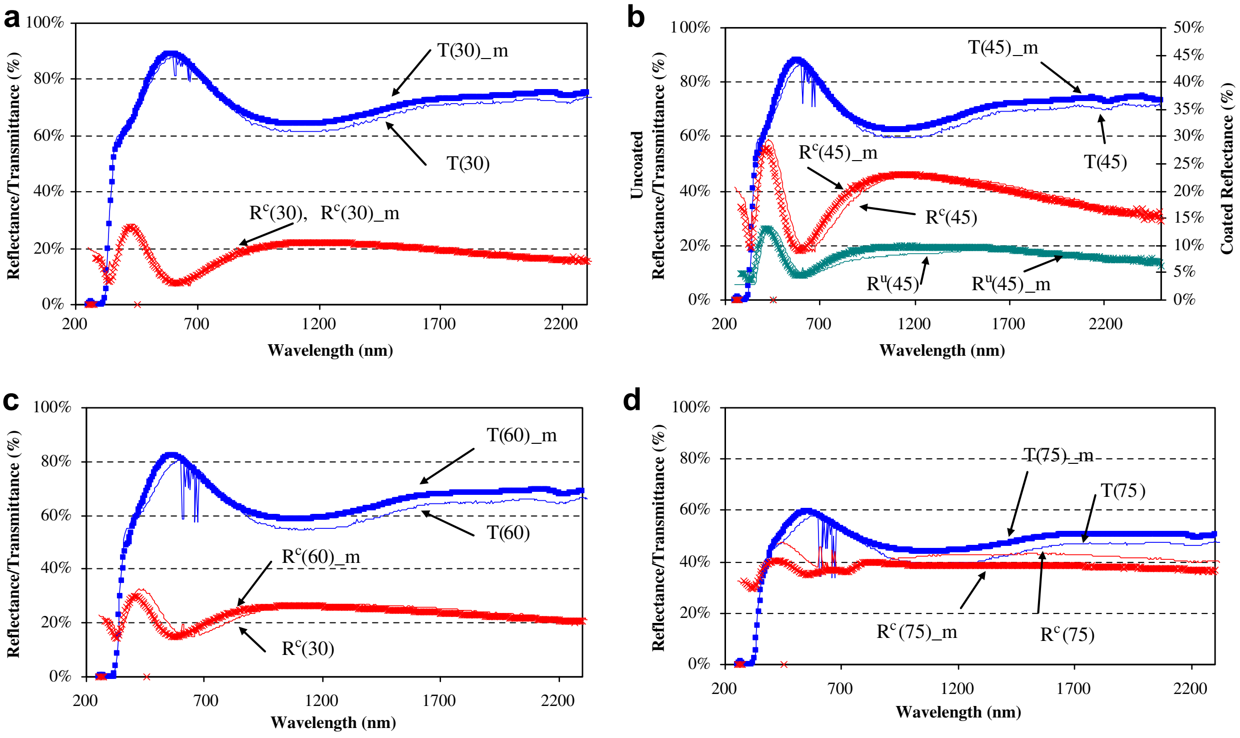

Fig. 6. Spectral transmissivities and reflectivities from the model versus measurement data (_m subscript) for several incident angles: (a) 30°, (b) 45°, (c) 60°, and (d) 70°.

validation to check the validity of the model when the values are calculated under oblique incident radiation.

5. Results and discussion

Selected data for this validation study have been the measured values of transmissivity and reflectivity for near normal incident radiation, s- and p-polarisation for 30°, 45°, 60° and 75° (Hutchins et al., 2001). The project samples that were finally used are the following: SnO_2/Ag/SnO_2/glass, TiN/glass, SnO_2/glass and conducting ITO/glass.

The comparative analyses of the modelled experimental results were developed at different levels. First of all, the

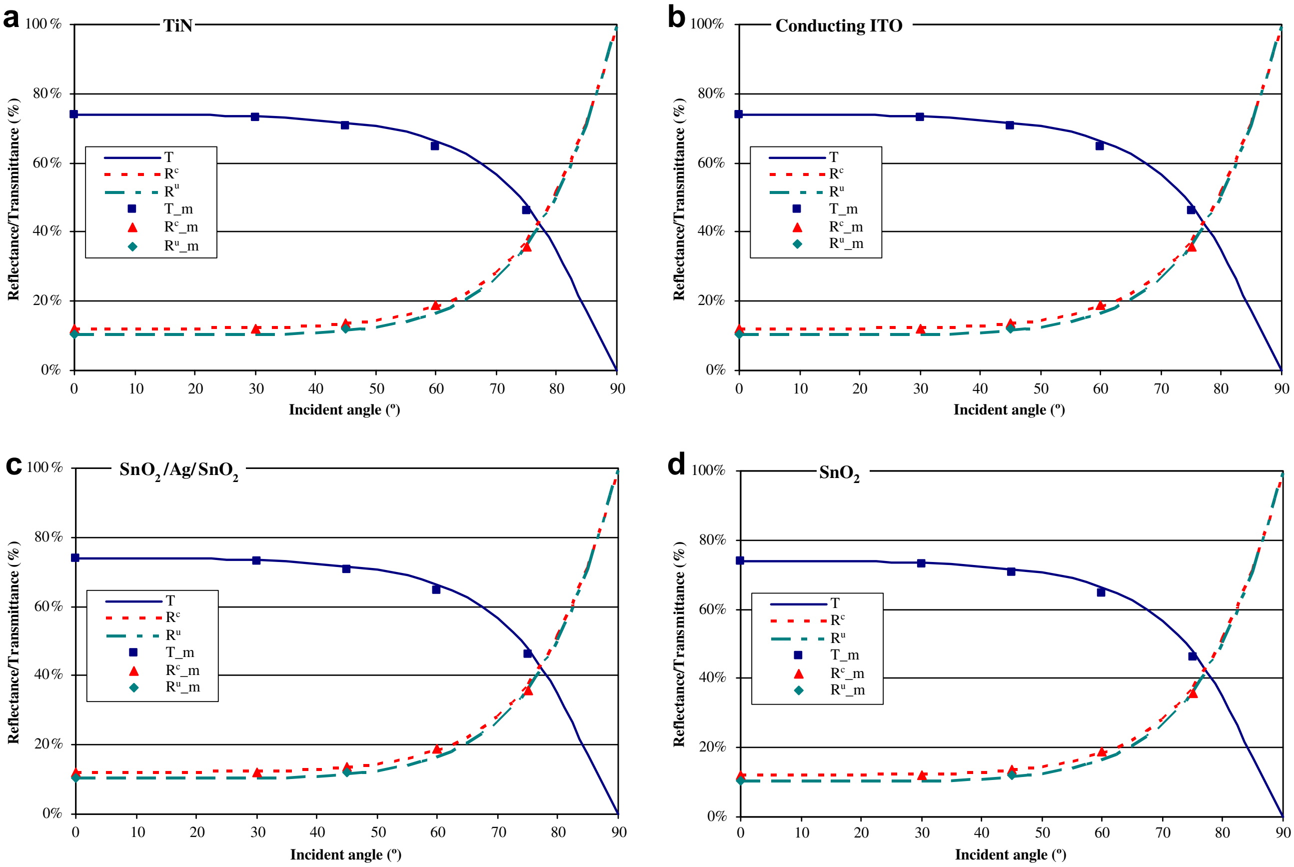

Fig. 7. 410-EN standard transmissivities and reflectivities from the model versus measured data (_m subscript) for several coatings: (a) TiN, (b) conducting ITO, (c) SnO_2/Ag/SnO_2, and (d) SnO_2.

Table 1
Absolute errors of the single-thin-film model over 4 studied samples

Samples		Absolute errors				Average relative error (%)
		30°	45°	60°	75°	
SnO_2/Ag/SnO_2	T	0.0025	0.0099	0.0333	0.0747	2.65
	R^c	0.0000	−0.0102	−0.0388	−0.0756	2.71
	R^u	–	−0.0137	–	–	0.69
TiN	T	0.0008	0.0023	0.0068	0.0129	0.50
	R^c	0.0052	0.0020	−0.0021	0.0018	0.24
	R^u	–	−0.0462	–	–	2.31
SnO_2	T	−0.0056	−0.0134	−0.0241	−0.0325	1.58
	R^c	0.0038	0.0046	0.0101	0.0401	1.34
	R^u	–	0.0021	–	–	0.10
Conducting ITO	T	0.0043	0.0104	0.0162	0.0178	1.00
	R^c	0.0014	−0.0009	−0.0048	0.0191	0.61
	R^u	–	−0.0063	–	–	0.31

Table 2
Single-thin-film versus hybrid equivalent model

Averaged errors			
Sample	Variable	One-thin-film (%)	Hybrid (%)
$SnO_2/Ag/SnO_2$	T	2.65	3.00
	R^c	2.71	3.40
	R^u	0.69	3.40
TiN	T	0.50	0.20
	R^c	0.24	0.30
	R^u	2.31	0.70
SnO_2	T	1.58	0.30
	R^c	1.34	0.20
	R^u	0.10	0.20
Conducting ITO	T	1.00	0.60
	R^c	0.61	0.40
	R^u	0.31	0.20

spectral performance for s-, p- and the average polarisation were obtained, with very satisfactory results, with average relative errors between 1% and 2%. The good performance reached for oblique angles (30°, 45°, 60° and 75°), which is the goal of the model, is shown in Fig. 6.

Integral properties are more useful for building energy consumption. The results obtained by using the EN-410 standard are shown in the Fig. 7. In these cases the results are even better than the spectral results due to the low weight of many of the wavelengths that do not perform well.

Table 1 shows the absolute errors (ΔR, and ΔT) and average relative errors ($\Delta R/R$ and $\Delta T/T$) for the selected samples. The absolute errors are practically negligible at low incident angles and increase as the angle increases, being lower than 0.07 for all cases.

In order to make a comparison with an alternative method, the *hybrid equivalent model algorithm* (Montecchi et al., 2001), which was widely validated during the ADOPT project, has been used. The comparison between the two models is shown in Table 2.

The errors of both methods have the same order of magnitude though they are smaller for the hybrid model (except for the first sample). Nevertheless, from the programming point of view, the proposed method shown in this paper is simpler than the hybrid model, because it uses only a thin-film. This way, only two optical parameters are required for each wavelength. Furthermore, the convergence process is guaranteed and the model can be used by an inexperienced user.

6. Conclusions

In this paper, a one-thin-film model developed to characterise the optical performance of any coated glazing is analysed. Furthermore, a method based on numerical optimisation has been successfully developed in order to find the adequate optical constants of the metallic thin film for any wavelength.

A first validation of the model has been performed using experimental information from the ADOPT project. This validation reveals that the average relative errors are smaller than 1% in most cases, being rarely higher than 2%. These results are comparable to the ones obtained by the hybrid equivalent method (Montecchi et al., 2001). The model described in this contribution has the advantage that it can be more readily implemented in computer software and it ensures the convergence of the optimisation process without user supervision.

Within the models validated in the frame of the ADOPT project, the empirical model developed by Roos et al. (2000), has the advantage of being easily updated with new standards and incorporated in any simulation software which does not need spectral information for glazings. Furthermore, it shows a very good accuracy. However, knowledge of the type of coating is needed for this empirical model to select the adequate parameters for the data. The model presented in this paper does not need any information about the coating, neither the material nor its thickness. Furthermore, it can be readily used in building simulation programs in which spectral information is required. In view of the promising results obtained and for future work, it will be interesting to extend the study using more experimental data in order to test the limits of this method.

Acknowledgements

The authors wish to thank the long term financial support received from the Commission of the European Union, throughout different programs and projects (WIS, REVIS, SOLAR CONTROL, ADOPT, SOLVENT, WINDAT), as well as the International Energy Agency for providing a discussion forum in its TASK 18. The authors also thank Ms. M. Molina Gutiérrez for her improvement of the English text.

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