MATHEMATICAL MODELS OF SOLAR ENERGY CONVERSION SYSTEMS

Viorel Badescu
Candida Oancea Institute, Polytechnic University of Bucharest, Romania

Keywords: photothermal conversion, photovoltaic conversion, photochemical conversion, thermodynamic models, detailed balance models.

Contents

Summary

Elementary concepts about modeling thermal radiation (with solar radiation as a particular case) are introduced. General aspects concerning the mathematical description of solar radiation concentration are treated. The basic physics necessary to describe mathematically the operation of photothermal, photovoltaic and photochemical devices, respectively, is briefly presented. Examples are given for models based on spectrally integrated energy fluxes or on detailed balance equations. The way of improving the models accuracy is emphasized and results obtained by using more detailed models are listed.

1. Introduction

A solar energy conversion system consists of a number of devices with different functions. The most important device is the absorber, where the received radiation energy is transformed into a different form of energy. The conversion system may, or may not, incorporate other devices. For example, some devices are used to diminish the energy losses from the absorber to the environment. Also, the radiation is sometimes concentrated before reaching the absorber, by using a device called radiation concentrator. Energy storage units as well as devices ensuring a better matching of the useful energy provided by the absorber to the user load may also be parts of the conversion system. However, specific to the solar energy conversion technology are the absorber and the concentrator. This work mainly focuses on the mathematical modeling of processes taking place in these two devices.

The solar energy absorbers may be academically divided into two categories: devices based on thermal processes and devices based on quantum processes, respectively.

In the first case, most part of the solar energy is transformed into internal energy of the body receiving radiation. This way of dealing with solar energy is called photothermal conversion. Very often the body receiving radiation is a metal or an alloy. The internal energy may be subsequently used directly (as in case of a device providing heat to an end-user), may be stored or may be transformed into mechanical, electrical or chemical work.

The absorbers based on quantum processes transform part of the energy of solar radiation directly into electrical energy (as it happens in a photovoltaic cell) or store that energy under the form of chemical energy (as it happens in case of water photo-dissociation into oxygen and hydrogen). The first process is called photovoltaic conversion while the second one is called photochemical conversion. Most photovoltaic devices are built with energy band gap materials like semiconductors. Photo-sensible substances are used within photochemical conversion devices.

There always exists a part of the incoming solar energy which cannot be converted directly into electrical or chemical energy and is dissipated as heat. Different design solutions are available to use that excess heat. There are some reasons why such kind of hybrid (combined) systems, which are able to generate simultaneously electrical (or chemical) and thermal energy or mechanical work, are attractive. First, many solar energy users require both kind of energies. Second, by extracting the heat from the device based on quantum processes (e.g. the solar cell) one improves its conversion efficiency. Hybrid systems are not treated here.

The mathematical description of solar energy conversion into other forms of useful energy requires understanding of how to model

- the incoming solar radiation as well as the radiation emitted by the absorber,
- the body receiving radiation and
- the interaction between the radiation and the receiving body.

In this work, the main concepts, parameters and principles used to model all these three aspects are briefly presented. First, a few elementary theoretical tools used in modeling thermal radiations (with solar radiation as a particular case) are introduced. Next, the general principles governing solar radiation concentration and the main associated parameters are presented. Finally, the basic physics necessary to describe mathematically the operation of photothermal, photovoltaic and photochemical devices, respectively, is briefly reviewed.

2. Properties of Radiation Fluxes

The spectrum of solar radiation just outside the atmosphere closely resembles the spectrum of a black body of temperature 5760 K. At ground level, the short wavelength radiation of solar origin consists of direct and diffuse radiation. There are many dips in the spectrum of the direct component, due to absorption by water vapor, oxygen and other gases in the atmosphere. The spectrum of the diffuse radiation has a narrower spread of wavelengths (or frequencies) and contains far less energy than that of the direct component. Many calculations can be made in an approximate manner using black body spectra rather than the correct solar spectrum. In fact, in any consideration of solar energy, the rather simple concept of the "black body" is very helpful: Its energy integrated over all wavelengths is simply a constant multiplied by the absolute temperature raised to the fourth power.

Most of the models presented in the next sections are based on balance equations at the level of solar energy conversion devices. These equations may involve photon energy, entropy or number fluxes. Some of these fluxes may be approximated by assuming they are emitted by black bodies but special assumptions should be adopted in case of the fluxes emitted by band-gap materials. Simple models for various photon fluxes emitted by black bodies and band-gap material are presented in this section.

2.1. Photons in Discrete Quantum States

The conversion of solar energy is always based on the interaction between the photons constituting solar radiation and the matter constituting the conversion devices. This matter mainly consists of fermions (for instance, electrons) and bosons (for instance, the phonons of the grid of a condensed body). The energy levels of these particles are quantified and transition between the energy levels is allowed just for particular values of the energy of the incoming photons. The photons having the appropriate energy are interacting with the conversion devices particles (i.e. they are absorbed) and the device is practically transparent for the other incoming photons. Also, the transitions of the device particles take place between quantified energy levels and the emitted photons have, accordingly, quantified energies. These emitted photons are characterized by quantified wavelengths, corresponding to the differences between the energy levels of the matter constituting the conversion device.

The electromagnetic radiation is often modeled as a photon gas, i.e. a system consisting of a mixture of photons of various wavelengths. One denotes by $P(N_1, N_2,...)$ the probability to find N_1 photons in quantum state 1, N_2 photons in quantum state 2 and so on. The following assumptions are usually adopted:

(i)the single quantum state probabilities $p(N_1)$, $p(N_2),...$, are independent, i.e.

$$P(N_1, N_2,...) = p\left(N_1\right)\cdot p(N_2)... \tag{1}$$

(ii)the probability that a new particle added to the system to be found in the quantum state j is independent of the number of particles already existing in that state. This means $p_j(N_j) = q_j^{N_j}$ where q_j is an undetermined positive number. Through the normalization condition one finds:

$$p_j(N_j) = (1-q_j)q_j^{N_j} \qquad \left(0 \le q_j \le 1\right) \tag{2}$$

These two hypotheses allow deriving all necessary concepts without adopting the assumption of thermodynamic equilibrium. The parameter q_j may be correlated to the mean occupation number n_j of the state j, if one takes account that:

$$n_j = \sum_{N_j=0}^{\infty} N_j p_j(N_j) = \sum_{N_j=0}^{\infty} N_j q_j^{N_j}(1-q_j) = \frac{q_j}{1-q_j} \tag{3}$$

The entropy S of the photon gas is given by

$$\begin{aligned} S &= k\sum_{N_1=0}^{\infty}...\sum_{N_j=0}^{\infty}...P\left(N_1, N_2,...\right)\ln P\left(N_1, N_2,...\right) \\ &= -k\sum_j\sum_{N_j=0}^{\infty}\left\{\left(1-q_j\right)q_j^{N_j}\ln\left[\left(1-q_j\right)q_j^{N_j}\right]\right\} \\ &= -k\sum_j\left[\left(1+n_j\right)\ln\left(1+n_j\right)-n_j\ln n_j\right] \end{aligned} \tag{4}$$

Here k is Boltzmann's constant.

2.2. Photons in Continuous Spectrum

When the distance between the photon energy levels is very small, the model of a continuous spectrum is often used. In this case the summation over quantum states is replaced by integration, which requires an expression for the number of photon quantum states in the frequency range $(\nu, \nu + d\nu)$ or, in other words, in the energy range $(e, e + de)$. Conversion between the frequency ν and the energy e may be easily obtained from $e = h\nu$ where h is Planck's constant. Sometimes $\omega \equiv 2\pi\nu$ is used as a frequency and the Planck relation becomes $e = \hbar\omega$ with $\hbar \equiv h/(2\pi)$.

One considers a volume V containing radiation. The refractive index of the medium inside the volume equals unity. A flux of radiation is incident on a surface element in the solid angle $d\Omega$ from a direction making the angle θ with the normal at the surface. The surface element may be part of the surface of the volume V or may be placed inside that volume. In the first case, the normal is oriented towards outside the volume. Then, the number of photon quantum states in the frequency or energy range is given by:

$$dN_v = \frac{d\Omega V \nu^2}{c^3} d\nu, \qquad dN_e = \frac{d\Omega V e^2}{h^3 c^3} de \qquad (5, 6)$$

where c is the speed of light. The number of photons in the frequency interval $(\nu, \nu + d\nu)$ is obtained from the density of quantum states dN_ν times the mean occupation number n_ν of the quantum state of frequency ν. The total number N of photons in the volume V is obtained through integration over all frequencies and the total solid angle:

$$N = V \iint \tilde{n}_\nu d\nu d\Omega \qquad \left(\tilde{n}_\nu \equiv \frac{l\nu^2}{c^3} n_\nu \right) \qquad (7,8)$$

Here $l = 1$ and $l = 2$ stand for polarized and unpolarized radiation, respectively. The internal energy U of the radiation is given by:

$$U = V \iint \tilde{u}_\nu d\nu d\Omega \qquad \left(\tilde{u}_\nu \equiv \frac{l\nu^2 h\nu}{c^3} n_\nu \right) \qquad (9,10)$$

Using (4) one obtains the entropy S of the radiation confined to the volume V:

$$S = V \iint \tilde{s}_\nu d\nu d\Omega \qquad \left(\tilde{s}_\nu \equiv \frac{lk\nu^2}{c^3} \left[\left(1 + n_\nu\right) \ln\left(1 + n_\nu\right) - n_\nu \ln n_\nu \right] \right) \qquad (11,12)$$

The quantities $\tilde{n}_\nu$, $\tilde{u}_\nu$ and $\tilde{s}_\nu$ are photon number, internal energy and entropy densities, respectively (Their units are: number of photons, energy unit or entropy unit, respectively, per unit volume, unit frequency and unit solid angle).

2.3. Properties of Photon Fluxes

The photons fluxes emitted or received by solar conversion devices are carrying various properties, such as number of particles, energy and entropy. The photon number flux density γ received by a Lambertian plane surface is given by

$$\gamma = \iint \Re_{N,\nu} \cos\theta d\nu d\Omega \qquad \left(\Re_{N,\nu} = c\tilde{n}_\nu = \frac{l\nu^2}{c^2} n_\nu \right) \qquad (13,14)$$

The radiation energy flux φ is given by:

$$\varphi = \iint \Re_{E,\nu} \cos\theta d\nu d\Omega \qquad \left(\Re_{E,\nu} = c\tilde{u}_\nu = \frac{lh\nu^3}{c^2} n_\nu \right) \qquad (15,16)$$

while the radiation entropy flux ψ is given by:

$$\psi = \iint \Re_{S,\nu} \cos\theta d\nu d\Omega \left(\Re_{S,\nu} = c\tilde{s}_\nu = \frac{lk\nu^2}{c^2} \left[\left(1+n_\nu\right) \ln\left(1+n_\nu\right) - n_\nu \ln n_\nu \right] \right) (17,18)$$

Here $\Re_{N,\nu}$, $\Re_{E,\nu}$ and $\Re_{S,\nu}$ are the photon number, the energy and the entropy spectral radiance, respectively. The factor $\cos\theta$ projects the plane surface area in such a way to be perpendicular on the propagation direction of the radiation. The light speed c takes account that the number of photons in the frequency range $\Delta\nu$ incident from the solid angle $d\Omega$ perpendicularly on the surface area ΔA during the time interval Δt is given by $\Re_{N,\nu} d\nu d\Omega \Delta A \Delta t = \tilde{n}_\nu d\nu d\Omega \Delta A (c\Delta t)$, where the radiation is contained by a cylinder whose axis length is $c\Delta t$. A similar argument applies in case of the energy and entropy fluxes.

In case of isotropic radiation, $\Re_{N,\nu}$, $\Re_{E,\nu}$ and $\Re_{S,\nu}$ do not depend on direction and

$$\gamma = B\int \Re_{N,\nu} d\nu, \qquad \varphi = B\int \Re_{E,\nu} d\nu, \qquad \psi = B\int \Re_{S,\nu} d\nu \qquad (19,20,21)$$

where

$$B \equiv \int \cos\theta d\Omega \qquad (22)$$

is the so called geometric (or view) factor, which captures the geometrical relation between the source and the receiver of radiation.

A common case corresponds to a spherical source of radiation (e.g. the Sun). One denotes by δ the half-angle of the cone subtending the sphere when viewed from the observer. The largest direct solar energy flux corresponds to the case when the center of the sphere is on the normal of the absorber surface. Only this case is considered in the present work. Then, after integration over the azimuth angle β and incidence (or zenith) angle α, one obtains the geometrical factor as a function of the half-angle δ:

$$\mathrm{B}(\delta) = \int_0^{2\pi} \mathrm{d}\beta \int_0^{\delta} \cos\alpha \sin\alpha \mathrm{d}\alpha = \pi \sin^2 \delta \tag{23}$$

In terms of the solid angle Ω subtended by the spherical radiation source, the same geometric factor B is given by:

$$\mathrm{B}(\Omega) = \Omega\left(1 - \frac{\Omega}{4\pi}\right) \tag{24}$$

Sometimes the source of radiation is a hemispherical dome ($\delta = \pi/2$). This happens for example in case of diffuse solar radiation received by a horizontal surface. In this case, after integration one finds $\mathrm{B} = \pi$.

2.4. Spectral Property Radiances for Blackbodies and Band-gap Materials

Many solar energy conversion devices involve radiation sources that may be described as blackbodies or band-gap materials. Generally, the radiation emitted by such bodies is characterized by the following simple expression for the mean occupation number n_ν of the quantum state of energy $\mathrm{h}\nu$:

$$\mathrm{n}_\nu = \frac{1}{\exp(\frac{\mathrm{h}\nu - \mu}{\mathrm{kT}}) - 1} \tag{25}$$

where T is the temperature of the body and μ is the chemical potential of the radiation. In case of blackbody radiation, $\mu = 0$. In case of a band-gap material (for instance, a semiconductor), $\mu = \mathrm{q}(\mathrm{E_{Fe}} - \mathrm{E_{Fh}})$ where $\mathrm{E_{Fe}}$ and $\mathrm{E_{Fh}}$ are the quasi-Fermi levels for electrons and holes, respectively. For a semiconductor solar cell the usual approximation is $\mathrm{E_{Fe}} - \mathrm{E_{Fh}} = \mathrm{V}$, where V is the voltage across the cell. Then, the Eq. (25) for $\mu = \mathrm{qV}$ becomes

$$\mathrm{n}_\nu = \frac{1}{\exp(\frac{\mathrm{h}\nu - \mathrm{qV}}{\mathrm{kT}}) - 1} \tag{26}$$

The Eqs. (25) and (26) may be used in Eqs. (14), (16) and (18) to compute the photon number, the energy and the entropy spectral radiances, respectively, for blackbodies or band-gap materials.

3. Concentration of Solar Radiation

A solution to increase the useful energy flux provided by the solar energy conversion system is to augment the surface area of the absorber. This way a larger amount of solar energy is collected. Another method to increase the collected solar energy is to keep the same absorber surface area and to concentrate the incoming solar radiation.

In many cases this second solution has the advantage that yields an increase of conversion efficiency and that the cost per unit surface area of the concentrating device is smaller than that of the absorber. Also, radiation concentration is used when a higher absorber temperature is wanted. Concentrating devices are shortly called concentrators. Adding a concentrator to the conversion system has some disadvantage, as for example the fact that only the direct component of the solar radiation is concentrated and the need to change concentrator orientation, due to the apparent Sun movement on the celestial vault. Also, the quality of concentrator’s mirror or lens is sometimes degrading faster in time than the quality of the absorber surface.

Two categories of solar concentrators are often used. In some concentrators the transversal surface area of the incident beam is diminished on two perpendicular directions. These devices may be called 3D concentrators.

The beam radiation is concentrated into a spot, which ideally reduced to a point. In other concentrators the transversal surface area is diminished on a single direction. These devices may be called linear or 2D concentrators. The beam radiation is concentrated into a strip, which ideally reduces to a line.

There is a maximum limit for solar radiation concentration. The first part of this section shows how this limit may be theoretically derived. Solar radiation concentration requires relatively large optical surfaces. Dioptric systems (lenses made of transparent materials, such as glass) are rarely used in practice due to their fragility and their relatively large weight and cost.

Catoptric systems (mirrors) are often used. The two most important parameters describing the performance of solar radiation concentration by mirrors are briefly introduced in the last part of this section.

-
-
-

Bibliography

Badescu V. (1998). Accurate upper bounds for the conversion efficiency of black-body radiation energy into work, *Physics Letters A* **244**, 31-34. [this paper shows the basic procedure to improve the accuracy of models treating solar energy conversion into mechanical work].

Badescu V. (2005). Spectrally and angularly selective photothermal and photovoltaic converters under one-sun illumination. *Journal of Physics D: Applied Physics* **38**, 2166-2172 [this paper proposes a new method to increase the performance of photothermal and photovoltaic conversion].

Badescu V., Landsberg P. T. (1993). Theory of some effects of photon recycling in semiconductors, *Semiconductor Science and Technology* **8**, 1267-76. [this paper is recommended for those readers interested to see how a more realistic model of photovoltaic cell operation may be developed].

Badescu V., Landsberg P. T. (1995). Statistical thermodynamic foundation for photovoltaic and photothermal conversion . I. Theory. *Journal of Applied Physics* **78** 2782-2792. [this paper uses a kinetic model based on Boltzmann equations to derive rigorously both the detailed balance equations and the thermodynamic formalism used in modeling photothermal and photovoltaic conversion].

Badescu V., Landsberg, P. T. (2000). Thermodynamics of solar energy conversion into work and some methods of analyzing solar cell efficiencies. Chapters 2 and 4 in *Thermodynamics of Energy Conversion and Transport*, Sieniutycz S., De Vos A. (Eds), New York: Springer, pp 14-48 and 72-105. [these two chapters present in a systematic way the bases of photothermal and photovoltaic conversion].

Bolton J. R. (1996) Solar photoproduction of hydrogen: a review, *Solar Energy* **57**, 37-50 [A complete summary of the science associated with one of the most promising photochemical conversion technology].

De Vos A. (1992). *Endoreversible Thermodynamics of Solar Energy Conversion*, New York: Oxford University Press [this book cover presents solar energy conversion starting from elementary principles].

Duffie J. A., Beckman W. A. (1991). *Solar Engineering of Thermal Processes*, Second Edition, New York: Wiley-Interscience. [influential book treating the photothermal conversion at engineering level].

Fahrenbruch A.L., R. H. Bube R.H. (1983). *Fundamentals of Solar Cells – Photovoltaic Solar Energy Conversion*, New York: Academic Press [authoritative book in the field of photovoltaic conversion].

Green, M. A. (1982). *Solar Cells: Operating Principles, Technology and System Applications*, New Jersey: Prentice-Hall [authoritative book in the field of photovoltaic conversion].

Hough T. P. (Ed.) (2006). *Solar Energy: New Research*, New York: Nova Science Publishers. [A compendium of technical articles on most types of solar energy conversion systems written by authoritative authors].

Landsberg P. T., Tonge G. (1980). Thermodynamic energy conversion efficiencies, *Journal of Applied Physics* **51,** R1. [a seminal paper treating the basic theoretical tools needed by modelers of solar energy conversion systems].

Landsberg P. T., Nussbaumer H., Willeke G. (1993). Band band impact ionization and solar cell efficiency, *Journal of Applied Physics* **74**, 1451-1452. [this seminal paper is recommended for those readers interested to see how a more realistic model of photovoltaic cell operation may be developed].

Landsberg P. T., Badescu V. (1998). Solar energy conversion: list of efficiencies and some theoretical considerations. Part I - Theoretical considerations, Part II - Results, *Progress in Quantum Electronics* **22**, 211-230 and **22**, 231-255. [an extended summary of theoretical and experimental results associated with photovoltaic conversion].

Markvart T., Landsberg P. T. (2002). Thermodynamics and reciprocity of solar energy conversion, *Physica E* **14**, 71-77. [this paper proposes a treatment based on irreversible thermodynamics for photochemical conversion].

Pleskov Y. V. (1990). *Solar Energy Conversion: A Photoelectrochemical Approach*. Berlin: Springer. [a readable introduction to photochemical conversion processes and technologies].

Shockley W., Queisser H. (1961). Detailed balance limit of efficiency of p-n junction solar cells, *Journal of Applied Physics* **32**, 510. [a seminal paper treating the application of detailed balance principle to solar cell efficiency calculation]

Winston R., Minano J. C., Benitez P. (2005). *Nonimaging Optics*, London: Elsevier Academic Press. [This book presents in a comprehensive and rigorous way the theory of solar energy concentrators].

Biographical Sketch

Viorel Badescu (born Bughea de Jos, Arges, Romania, September 24, 1953) is professor of engineering thermodynamics at Polytechnic University of Bucharest. His mainstream scientific contributions consist of about two hundreds papers and several books related to statistical physics and thermodynamics, the physics of semiconductors and various aspects of terrestrial and space solar energy applications. Also, he has theorized on present-day Mars meteorology and Mars terraforming and on several macro-engineering projects. He is reviewer or Associate Editor of more than twenty international journals and member of eight scientific societies among which the International Solar Energy Society and the European Astronomical Society. He received four awards among which the Romanian Academy Prize for Physics in 1979.