Project PD 53/2022

project code: PN-III-P1-1.1-PD-2021-0208

Contracting authority: Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI.

Acronym and project title: **POSOMAN**

"The influence of pollution on solar cell manufacturing technologies"

SCIENTIFIC REPORT STAGE 2 (1.01.2023 - 31.12.2023)

The four activities engaged for Stage 2: Sun radiation measurements and estimated/calculated attenuation (committed completion date 31.12.2023) were completed according to the Project Implementation Plan in Annex II to financing contract no. PD 53/2022, namely:

Activity 2.1. *Flux radiation measurements in the atmosphere during different environmental and seasonal conditions-100%*

Activity 2.2. *Study of radiance attenuation-100%*

Activity 2.3. *Finding the optoelectronic parameters variation of existing commercial solar cells i.e. solar cells efficiency under different media stress conditions in the atmosphere - 100%*

Activity 2.4 *Experimental and numerical estimation of the optoelectronic parameters variation of existing commercial solar cells i.e. solar cells efficiency under interaction with high energy particles in outer space - 100%.*

In order to evaluate the sun **radiation effects on different materials**, different numerical models have been set-up in COMSOL using different geometries, modules and features: Heat Transfer in Solids, External Radiation Source, Multiband Emissivity etc. Preliminary results of three of the heating models studied in COMSOL are presented.

Initial temperature, T_0=273 K, and direct normal radiation of 4.57 kWh/m²/day are the same in all the three models. Features, analytical functions, variables, source equation, materials, boundry conditions and other parameters and conditions are different for each model.

The aim is to identify influences of materials and environmental conditions on the heating effects under sun radiation. Model 3 takes into account the emissivity of the materials.

- model 1: heating temperatures and heat flux in materials used in construction exposed to heating energy of sun radiation; T max-heating=293 K (Figure 1)

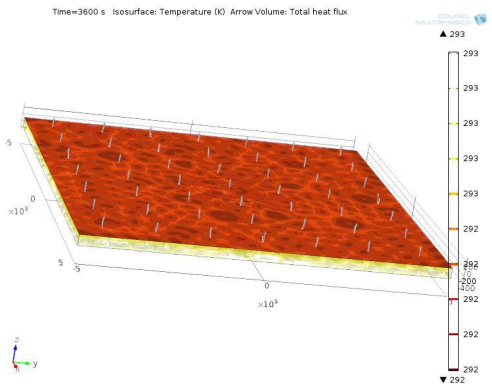


Figure 1. Heating effects on Materials: concrete/lime

- model 2: heating temperatures and heat flux in the sand exposed to the sun radiation and the sand surface emissivities; Tmax-heating = 366 K (Figure 2)

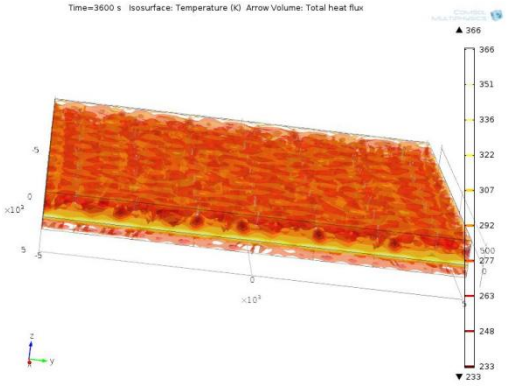
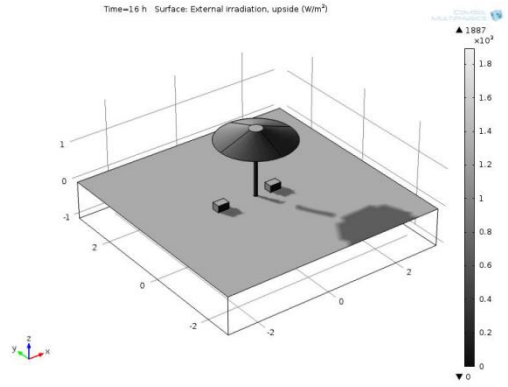
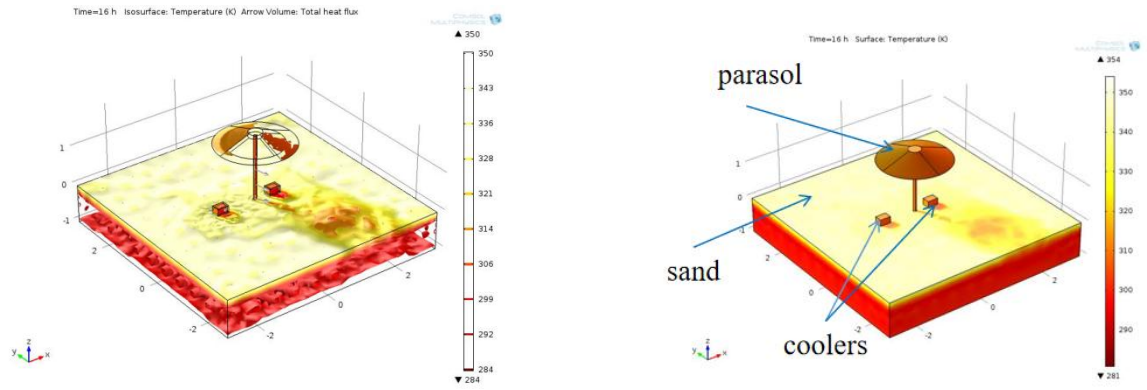


Figure 2. Heating effects on Materials: concrete/air

- model 3: heating temperatures and heat flux in the sand exposed to the sun radiation and the sand surface emissivities with coolers and shades influences: Tmax-heating = 350 K; External irradiation upside = $1887 \cdot 10^3$ W/m^2



(a)

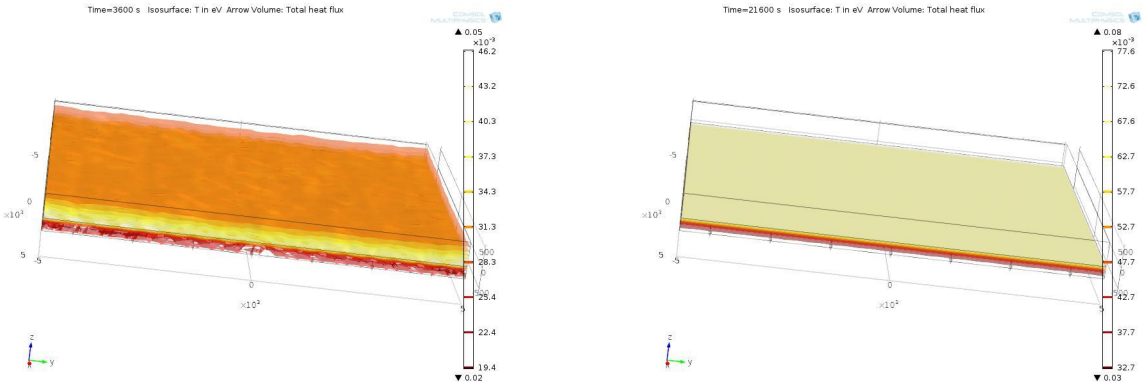


(b) (c)

Figure 3. Heating effects on materials: sand/aluminum/acrylic plastic: sand emissivity (a); isosurface (b); surface temperature (c)

The goal of the study is to set-up a numerical model that can be used for a variety of materials and situations specific to a certain urban area. The preliminary results demonstrate the possibility of creating such numerical models, and an optimization analysis will be carried out after the completion and validation of each of the models.

Furthermore, simulations were conducted to evaluate the **effects of the solar radiation on materials in terms of energy** (Figure 4.). 1 eV is the amount of energy gained by the charge of an electron moved across an electric potential difference of one volt. In other words, an electronvolt is 1 volt (1 joule per coulomb) multiplied by the electron charge (1 e, or $1.602176565(35)\times10^{-19}$ C). 1 kelvin [K] = 8.61732814974056E-05 electron-volt [eV].

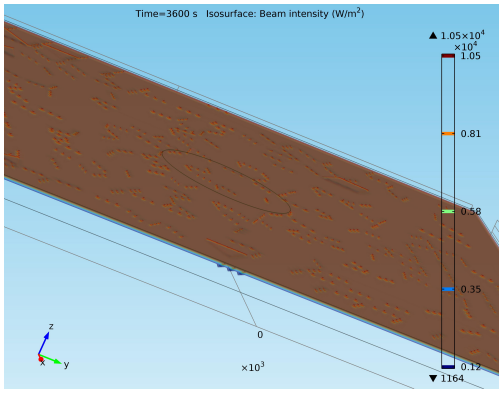


(a) (b)

Figure 4. Thermal effects induced in silica and the surrounding air after 3600 s (a) and 21600 s (b) of exposure to sun radiation

Different numerical models for simulation with Finite Element in COMSOL have been set-up under this project. The next step is to acquire data on sun radiation evolution for implementation in theparameters and used in the simulations.

Radiance attenuation was studied with simulation Finite Element Method in COMSOL based on numerical model developed in the research work under POSOMAN project. The 3D, 2D and 1D plots generated provide information on the influences of the particles deposited on the solar cell surface on the sun radiation intensity (Figure 5 a-e).



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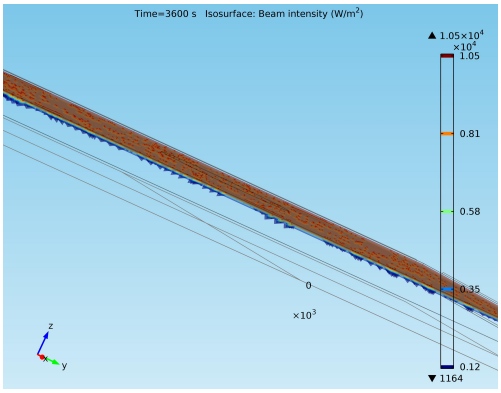

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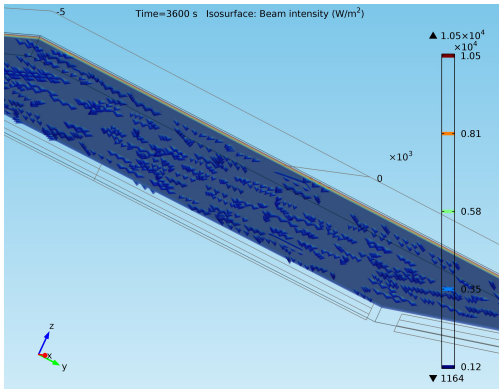

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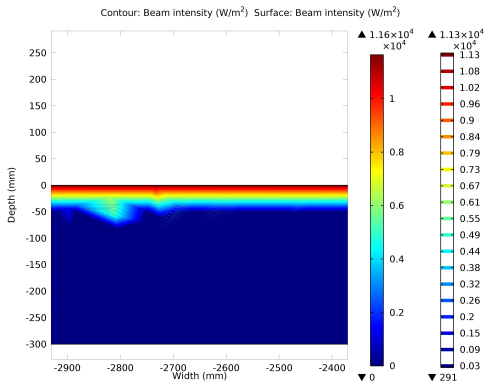

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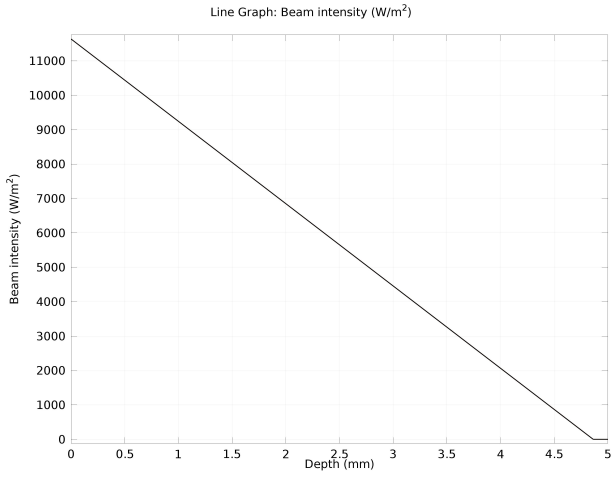


(e)

Figure 5. Sun radiation attenuation due to metallic impurities deposited on a substrate (solar cell): 3D Isosurface Plots (a-c); 2D cut plane xOz plot (d) and 1D plot beam intensity variation in depth of the material (e)

The **optoelectronic parameters** are material characteristics that change with the material state including impurities added and their interactions with the substrate. An experiment on Ag and Cu thin films obtained by PLD (Pulsed Laser Deposition) on glass substrate simulates the conductive components in a solar cell. Both layers were exposed to organic compound with buffer aqueous solution and the results showed high damage on the copper thin layer compared to Ag. The experiment was repeated on PLD obtained Ag/Cu and the quality of Cu thin layer was protected by the Ag thin layer. The results will be sent for publication beginning with February 2024 acknowledging the POSOMAN project.

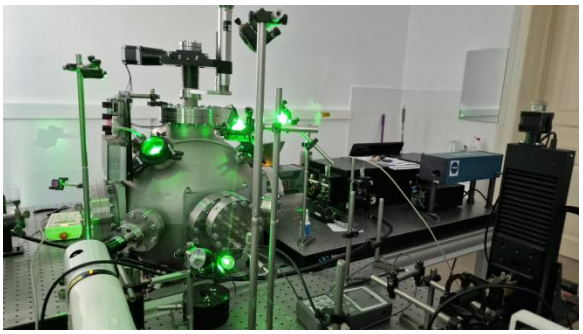
SPN1 Sunshine Pyranometer (Figure 5) was acquired with funding from the project for flux radiation measurements in the atmosphere.

The measurements with the SPN1 Pyranometer will start in January 2024 in order to compare the results obtained with the numerical simulations conducted in COMSOL and for **evaluation of changes of optoelectronic parameters of solar cells** in connection with measured sun radiation.

Figure 6. SPN1 Pyranometer

The SPN1 Pyranometer measures Global (Total) and Diffuse Radiation (W/cm^2) and Sunshine Duration – in one instrument with a WMO sunshine threshold of 120 W.m^{-2} direct beam. The instrument works at any latitude.

The study on solar cells related to stage 3 of the project has already been started. Thin films of materials obtained by PLD technique from biocomposites (hemp stalk and oyster shell) used as target were analyzed regarding their suitability for solar cells [1,2].



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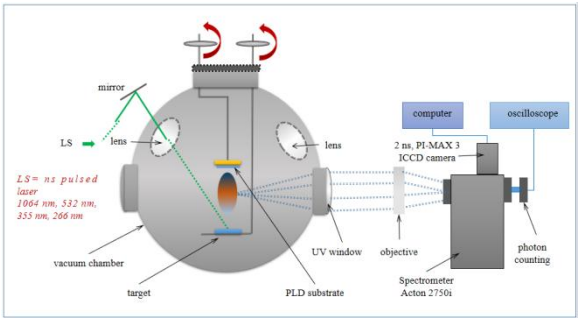

(b)

Figure 7. Experimental set up installation connected to the laser system YG 981E/IR-10 (a) and the schematic representation (b)

The thin films were obtained by the Pulsed Laser Deposition technique (PLD) using a 532 nm wavelength and 150 mJ/pulse laser beam, 10 ns pulse width, 10 Hz repetition rate.

(a) (b)

Figure 8. PLD techique (a) and thin film obtained from hemp stalk (b)

The results and discussions are reported by Cocean et al, 2023 [1]. Important to mention is the transfer of identical material as the hemp stalk target: lignin, cellulose; hemicellulose, p-cumaric and ferulic acids, starch, wax etc. (Figure 9). All these components are chemical structures with p-π conjugated bonds that recommend the material as solar cells components [1].

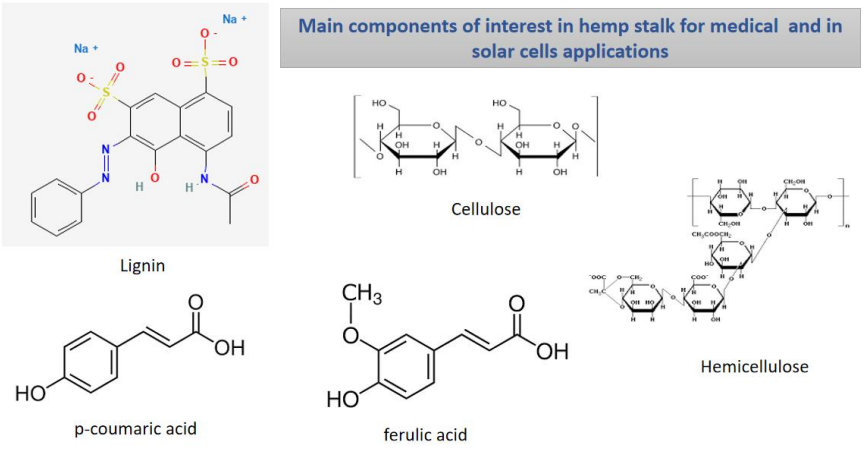

Figure 9. Main components in hemp stalk transferred as nano-components of thin film produced by PLD technique applied to the hemp stalk target

Conclusions:

The numerical models developed in COMSOL will contribute to the analysis of thermal and energetic absorption effects under sun radiation as well to the study of materials emissivity. Radiance attenuation due to particulate matter deposited on materials surface was studied with numerical model developed in COMSOL. In addition to the numerical simulation, sun radiation measurements are now available with the new **SPN1 Sunshine Pyranometer** acquired through the POSOMAN, PD53/2022 project. Thin films fabricated with the PLD technique from biocomposite materials are potential candidates to be included as components in the solar cells structure.

REFERENCES:

[1] Cocean, A.; Cocean, G.; Diaconu, M.; Garofalide, S.; Husanu, F.; Munteanu, B.S.; Cimpoesu, N.; Motrescu, I.; Puiu, I.; Postolachi, C.; Cocean, I. and Gurlui, S. Nano-Biocomposite Materials Obtained from Laser Ablation of Hemp Stalks for Medical Applications and Potential Component in New Solar Cells. Int. J. Mol. Sci. 2023, 24, 3892. https://doi.org/10.3390/ijms24043892

[2] Cocean, G.; Cocean, A.; Garofalide, S.; Pelin, V.; Munteanu, B.S.; Pricop, D.A.; Motrescu, I.; Dimitriu, D.G.; Cocean, I.; Gurlui, S. Dual-Pulsed Laser Ablation of Oyster Shell Producing Novel Thin Layers Deposed to Saccharomyces cerevisiae. Polymers 2023, 15, 3953. https://doi.org/10.3390/polym15193953

DELIVERABLES/ LIVRABILE:

4 ISI Papers:

1. Cocean, A.; Cocean, G.; Diaconu, M.; Garofalide, S.; Husanu, F.; Munteanu, B.S.; Cimpoesu, N.; Motrescu, I.; Puiu, I.; Postolachi, C.; Cocean, I. and Gurlui, S. Nano-Biocomposite Materials Obtained from Laser Ablation of Hemp Stalks for Medical Applications and Potential Component in New Solar Cells. Int. J. Mol. Sci. 2023, 24, 3892. https://doi.org/10.3390/ijms24043892
2. Cocean, G.; Cocean, A.; Garofalide, S.; Pelin, V.; Munteanu, B.S.; Pricop, D.A.; Motrescu, I.; Dimitriu, D.G.; Cocean, I.; Gurlui, S. Dual-Pulsed Laser Ablation of Oyster Shell Producing Novel Thin Layers Deposed to Saccharomyces cerevisiae. Polymers 2023, 15, 3953. https://doi.org/10.3390/polym15193953

3. Diaconu, M.; Garofalide, S.; Cocean, G.; Cocean, A.; Pricop, D. A.; Cocean, I. and Gurlui, S. Physico-Chemical Degradation of Some Land-Fill Wastes Contaminating on Surface and Ground Surrounding Waters, INTERNATIONAL JOURNAL OF CONSERVATION SCIENCE, ISSN: 2067-533X, Volume 14, Issue 3, July-September 2023: 1045-1056, DOI: 10.36868/IJCS.2023.03.17

4. Balbarau, A.; Ivanescu, L.M.; Martinescu, G.; Rîmbu, C.M.; Acatrinei, D.; Lazar, M.; Cocean, I.; Gurlui, S.; Cocean, A.; Miron, L. Septicemic Outbreak in A Rainbow Trout Intensive Aquaculture System: Clinical Finds, Etiological Agents, and Predisposing Factors. Life 2023, 13, 2083. https://doi.org/10.3390/life13102083

Conferences:

1. Alexandru Cocean, Georgiana Cocean, Silvia Garofalide, Vasile Pelin, Dana Angelica Pricop, Bogdanel Silvestru Munteanu, Nicanor Cimpoesu, Dan Gheorghe Dimitriu, Iuliana Cocean and Silviu Gurlui, Numerical simulation in assisting the experimental study as a tool for estimating the working parameters, anticipating and explaining the experimental results. COMSOL Multiphysics and Gaussian 6 software, Conferința FTEM (Fizica și Tehnologiile Educaționale Moderne) 20 mai 2023, http://ftem.faculty.ro/
2. Georgiana Cocean, Alexandru Cocean, Silvia Garofalide, Cristina Postolachi, Maria Diaconu, Francisca Husanu, Bogdanel Silvestru Munteanu, Nicanor Cimpoesu, Iuliana Motrescu, Ioan Puiu, Iuliana Cocean and Silviu Gurlui, Hemp stalk components transfer into composite nanostructures under high power pulsed laser ablation and deposition to produce functional materials, Conferința FTEM (Fizica și Tehnologiile Educaționale Moderne) 20 mai 2023, http://ftem.faculty.ro/
3. Daniela Pricop, Silvia Garofalide, Alexandru Cocean, Iuliana Cocean, Vasile Pelin, Silviu Gurlui, Historical buildings degradation as an effect of chemical contaminants from anthropogenic pollution sources, Conferința FTEM (Fizica și Tehnologiile Educaționale Moderne) 20 mai 2023, http://ftem.faculty.ro/
4. Cocean, A.; Postolachi, C.; Cocean, G.; Garofalide, S.; Diaconu, M.; Pelin, V.; Pricop, D.A.; Munteanu, B.S.; Motrescu, I.; Dimitriu, D.; Cocean, I. and Gurlui, S.; Detection of IR vibration bands in environmental analysis using GAUSSIAN 6 software, 4th International Workshop Advances on Photocatalysis (https://photocatalysis-workshop.eu/), 25-28 iulie 2023, online poster session (https://photocatalysis-workshop.eu/program/).

5. Cocean, G.; Cocean, A.; Postolachi, C.; Garofalide, S.; Pricop, D.A.; Munteanu, B.S.;Cocean, I.; Gurlui, S.; Saccharomyces cerevisiae and Fourier Transform Infrared Spectroscopy technique used to identify photo-chemical processes during laser ablation of hemp stalk, 4th International Workshop Advances on Photocatalysis (https://photocatalysis-workshop.eu/), 25-28 iulie 2023, online poster session (https://photocatalysis-workshop.eu/program/).
6. Postolachi, C.; Cocean, A.; Cocean, G.; Garofalide, S.; Pricop, D.A.; Munteanu, B.S.; Cimpoesu, N.; Motrescu, I.; Cocean, I.; Gurlui, S.; High pulsed laser energy to produce structural morphology of thin layers for green chemical processes, 4th International Workshop Advances on Photocatalysis (https://photocatalysis-workshop.eu/), 25-28 iulie 2023, online poster session (https://photocatalysis-workshop.eu/program/).
7. Cocean, A.; Motrescu, I.; Bulai, G.;, Garofalide, S.;, Pricop,D.; Pelin, V.; Cocean, G.; Diaconu, M.; Postolachi, C.; Husanu, F.; Pata, D.; Ababei, R.; Munteanu, B.; Cimpoesu, N.; Puiu, I.; Dimitriu, D.; Cocean, I.;Gurlui, S. Natural and anthropogenic phenomena that have played an important role in Romania in the last 5 years, European Lidar Conference ELC 2023,Cluj-Napoca, Romania, 13.09.2023-15.09.2023, https://enviro.ubbcluj.ro/european-lidar-conference-2023/ - prezentare Silviu Gurlui
8. ZILELE ACADEMICE IEŞENE, Ediţia a XXXVIII-a, Sesiunea științifică națională Vectori ai dezvoltării rurale în Regiunea Nord-Est a României (ediția a III-a) Sisteme agroalimentare durabile 12 octombrie 2023, *Alexandru Cocean, Georgiana Cocean, Cristina Postolachi, Silvia Garofalide, Diana Manuela Lina, Vasile Pelin, Maria Diaconu, Daniela Angelica Pricop, Răzvan Ababei, Dan Gheorghe Dimitriu, Bogdănel Silvestru Munteanu, Georgiana Bulai, Nicanor Cimpoeşu, Iuliana Motrescu, Ioan Puiu, Iuliana Cocean and Silviu Gurlui, Tehnologia de vârf bazată pe interacțiunea laserului cu materia implicată în dezvoltarea economiei rurale. Aplicabilitatea acesteia pe termen scurt și pe termen lung /Cutting-edge technology based on the interaction of laser with matter involved in the development of rural economy. Its short-term and long-term applicability*; Sesiunea științifică a avut loc online, în data de 12 octombrie 2023, între orele 9:30 – 16:30, pe platforma Zoom. https://us02web.zoom.us/j/83863323372?pwd=UDNmV1NJM3F5eEJ4SHR0Y1h1cFExZz09; Meeting ID: 838 6332 3372; Passcode: 941046-prezentare Iuliana Cocean
9. S. Garofalide, A. Cocean, G. Cocean, D.A. Pricop, R. Ababei, C. Postolachi, V. Pelin, I. Cocean, L. Leontie, S. Gurlui, *Understanding and Mitigating Urban Heat Island Effect,*

ICPAM-15; PAMS-6; November 19-26, 2023; Sharm El Sheikh, Egypt, https://icpams.com/main/programme-pams/

10. Georgiana Cocean, Alexandru Cocean, Cristina Postolachi, Silvia Garofalide, Maria Diaconu, Daniela Angelica Pricop, Razvan Ababei, Bogdănel Silvestru Munteanu, Georgiana Bulai, Nicanor Cimpoesu, Iuliana Motrescu, Vasile Pelin, Dan Gheorghe Dimitriu, Iuliana Cocean and Silviu Gurlui, Nanomaterials produced by laser techniques for TDD applications, *ICPAM-15; PAMS-6*; November 19-26, 2023; Sharm El Sheikh, Egypt, https://icpams.com/main/programme-pams/
11. Cristina Postolachi, Alexandru Cocean, Georgiana Cocean, Silvia Garofalide, Daniela Angelica Pricop, Bogdănel Silvestru Munteanu, Georgiana Bulai, Iuliana Motrescu, Vasile Pelin, Iuliana Cocean and Silviu Gurlui, Study of nano- and micro-particulate structure of the silver thin films deposited by high-energy pulsed laser ablation, *ICPAM-15; PAMS-6*; November 19-26, 2023; Sharm El Sheikh, Egypt, https://icpams.com/main/programme-pams/
12. Daniela Angelica Pricop, Alexandru Cocean, Georgiana Cocean, Cristina Postolachi, Silvia Garofalide, Georgiana Bulai, Laura Ursu, Vasile Pelin, Iuliana Cocean and Silviu Gurlui, Aerosol heavy metals photdetection techniques using novel gold nanoparticles systems coated with chitosan and lipids, *ICPAM-15; PAMS-6*; November 19-26, 2023; Sharm El Sheikh, Egypt, https://icpams.com/main/programme-pams/

SUMMARY OF THE SCIENTIFIC REPORT PROJECT PD53/2022-Stage 2/2023

Based on the numerical models developed, finite element simulation analyzes were carried out in COMSOL of the effects produced by solar radiation, including radiation attenuation. The models will also be used for the measurements that will be made with the newly purchased **SPN1 Sunshine Pyranometer**. It will thus be possible to analyze the effects induced by pollutants as well as the variation of solar radiation on the efficiency of solar cells and the materials used. The measurements will also be used as parameters in the experimental analysis. The development of new materials, composite polymer materials, with the potential to be included in the construction of solar cells was also addressed. Thus, thin layers were produced by the PLD (Pulsed Laser Deposition) method applied to natural biocomposites rich in polymeric constituents with a structure suitable for solar cells materials. A number of 4 ISI articles were published and 12 scientific communications to international and national conferences.

MAIN CONCLUSIONS:

1. The numerical models developed in COMSOL will contribute to the analysis of thermal and energetic absorption effects under sun radiation as well to the study of materials emissivity. Radiance attenuation due to particulate matter deposited on materials surface was studied with numerical model developped in COMSOL.
2. In addition to the numerical simulation, sun radiation measurements are now available with the new **SPN1 Sunshine Pyranometer** acquired through the POSOMAN, PD53/2022 project.
3. Thin films fabricated with the PLD technique from biocomposite materials are potential candidates to be included as components in the solar cells structure.

Director Proiect,

COCEAN Alexandru