Short Scientific report on the implementation of the project
PN-III-P2-2.1-PED2019-3970 (contract no. 357PED/2020) entitled
"Mitigation of Risk Factors for Public Health, Represented by Bio-Chemical Contaminants in Food and Pharma Packaging from Recycled Sources by A New Methodology Based on Spectral Analysis in Thz Domain – THzPET", Phase 2-2021

*Main objectives of phase 2*:

- Research related to optimal distribution and dispersion of THz signals on different samples of packaging at both plastic surface and bulk level;
- Development of test method by molecular dynamics simulation and cross-experiments for pattern recognition of contaminants in PET packaging.

Nowadays, polyethylene terephthalic acid (PET), the main component of plastic packaging materials with around 70 million tons being manufactured every year, is intensely used in a lot of applications, such as textiles, food and pharmaceutical industries. PET materials are single-used and are not degraded by microorganism, being estimated that from 359 million tons of plastics produced globally per year, 150–200 million tons accumulate in natural habitats.[1,2] As a solution for this important issue, in some packaging technologies, secondary recycled PET is used. Unfortunately, since there is no control over the waste PET source, and are often collected from some common city or industrial garbage dumps, secondary recycled PET can contain chemical and/or biological contaminants.[3,4] According to the literature data, there are over 175 potentially hazardous substances (alone or mixtures) legally used in the production of food/pharmaceutics contact materials that can be transferred towards packing, a high risk factor for public health.[4] The responsible authorities monitor the types of residues present in foods and drugs, but there is no actual laboratory methodology focused on chemical and biological contaminants in packaging.

Terahertz (THz) spectroscopy is an emerging technology that brings a number of technical breakthroughs in several scientific applications.[5] This new technique has gained considerable attention as a method for studying properties of various materials, based on its key features, such as: non-invasive and non-ionizing properties, phase-sensitive to polar compounds, selectivity to numerous organic molecules through particular absorption and dispersion, unique spectral feature used to recognize molecules in the THz range by assessing their specific spectral signatures, high spatial resolution capabilities, coherent detection and ability to penetrate nonpolar molecules.[6] Due to these unique properties, THz can be seen as a valuable technique in a variety of fields: chemistry, materials sciences, engineering and medicine.[7] But, compared with Raman and Infrared (IR) spectroscopy, the development of approaches for generating, manipulating, and detecting terahertz radiation are insufficiently studied.[8]

*Main activities performed in phase 2:*

- The formulated plastic samples from P1 were submitted for THz and ATR-IR spectroscopy (CO), according to pre-defined protocols.

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[1] M. O'Reilly, J. Stubbe, *Biochemistry*. 59, 25, 2316–2318, 2020.
[2] V. Tournier, C.M. Topham, A. Gilles, A. et al. *Nature*. 580, 216–219, 2020.
[3] H. Widén, A. Leufvén, T. Nielsen, *Food Addit Contam.* 22, 681-92, 2005.
[4] B. Geueke, C.C. Wagner, J. Muncke, *Food Addit Contam Part A Chem Anal Control Expo Risk Assess*. 31, 1438-50, 2014.
[5] M.B. Almeida, L. Schiavo, E. Esmanhoto, et al. *Braz Arch Biol Technol*. 64, e21200770, 2021.
[6] M. Danciu, T. Alexa-Stratulat, C. Stefanescu, et al. *Materials*. 12, 1519, 2019.
[7] J. Neu, C. A. Schmuttenmaer, *Journal of Applied Physics*, 124, 231101, 2018.
[8] W. Ghann, J. Uddin, *IntechOpen*. 1, 1-20, 2017.

- The samples were contaminated with protein solutions for simulation of the presence of biological contaminants. The contamination was performed using quantified protein solution added in droplets on the clean, decontaminated PET samples, oven dried and kept in protective environment until the analysis.
- The contaminated samples were analyzed using the same settings as the bare samples by THz and ATR-IR spectroscopy (CO). THz (using Terapulse 4000 Pulsed Portable Terahertz Spectrometer) and IR spectroscopy (using Spectrometer FT-IT Nicolet Summit Pro equipped with Everest attenuated total reflectance accessory) have been used to analyze the bare composite materials and the protein solution contaminated samples.
  The flowchart for these activities is presented in Figure 1.

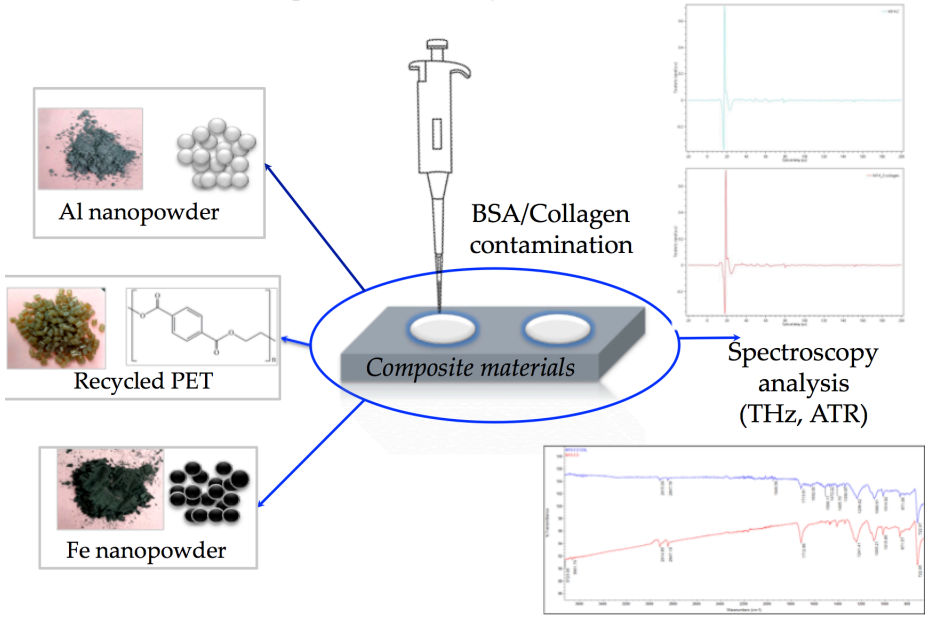


*Figure 1. Flowchart for the performed activities in phase 2*

Comparing the spectra obtain for simple materials and contaminated ones, significant differences have been observed, meaning that TDTTS and ATR-IR are promising techniques for identification of potential biochemical contaminates on recycled PET.

*Conclusion*

The deliverables associated the objective of phase 2:

- THz optical properties of packaging at both plastic surface and bulk level;
- Data processing methods for time-domain response;
- Identification of chemical and/or physical patterns at THz on experimental samples;
- Simulations on molecular dynamics in Gromacs package;
- Experimental procedure for relating molecular dynamics with chemical and/or physical patterns;
- Classification algorithm in THz domain and Database of contaminants features;
- 3 poster presentations at national/international conferences;
- Best Young Scientist Poster Communication (Offered by Romanian International Chapter of ACS);
- 2 papers under evaluation;
- 1 activity report.