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 1-2020

## *Main objective of phase 1 – R&D related to most adequate formulation for THz time-domain spectroscopy / method and equipment for selective evaluation of PET packaging*

Plastic materials currently have multiple uses and are a recoverable resource, beneficial to the environment and with a positive effect on the economy, through recycling programs. However, the technology that deals with the sorting of recyclable plastic faces a challenge given the inability to sort the entire mass of plastic products, thus hindering the optimal recycling process [1]. Manufacturers of food-contact articles made from recycled plastic are responsible for ensuring that, like virgin material, recycled material is of suitable purity for its intended use, European Food Contact Materials Legislation - Recycled plastic: (EC) No. 282/2008. Any secondary recycling process may be inappropriate for the production of food-contact articles, particularly because the recycler had little or no control over the waste stream entering the recycling facility, i.e. the waste PET source can be some common city or industrial garbage dumps, where the contamination probability is high; or, even if selective collected, some of PET packaging could have been used for storage of pesticides or automotive chemicals etc. Moreover, along with the chemical contaminants, the biological contaminants pose a threat against human health. Even in the conditions of harsh manipulation of PET residues, microbiological contamination can occur and in time could determine health issues [2 3 4].

Currently, multiple non-destructive methods are used to analyze various properties of materials. Much of the existing technology uses for evaluation the interaction between materials and electromagnetic radiation. Starting with gamma radiation and ending with radio waves, different spectral bands are used in applications on quantitative and qualitative analysis of materials. However, a certain part of the electromagnetic spectrum has remained unexplored for many years, which until the late 1980s was called the "terahertz gap" due to the difficulty in developing suitable sources and detectors [5].

THz waves have the following characteristics: non-ionizing and non-invasive (minimal effects on the human body); easily penetrable for many types of materials such as plastic, paper, wood, leather and have a lower penetration rate than microwave radiation. THz radiation has a high degree of water absorption and metals, a high degree of reflection and is sensitive to various resonance phenomena (vibration, rotation, translation, etc.) [6].

In the last decade, time-domain terahertz transmission spectroscopy (TDTTS) has become a powerful method for studying properties of various materials, due to its advantages as: penetration of a wide variety of non-conducting materials; sensitive to charge carriers; selective to numerous organic molecules through particular absorption and dispersion; no need for a coupling medium and low photon energies (4meV/1THz). TDTTS operates with sub-picosecond pulses of electromagnetic radiation, bridging a large frequency gap between microwave and conventional infrared spectroscopy. Materials or biological structures have their intrinsic THz spectra in the absorption and the refractive index, called as "fingerprint" THz spectra, bands of which originate in intermolecular and intramolecular vibrations [7].

The novelty of the proposed approach lies in the TDTTS adaptation as consistent way of emphasizing residual ingredients in e.g. PET packaging, technological issues or physical defects at micro-scale, due to molecular dynamics and intermolecular interactions between e.g. contaminants and polymer. In addition to bulk phonon modes, surface phonons and adsorbate-surface interactions can be measured, giving information exactly on food-contact surfaces.

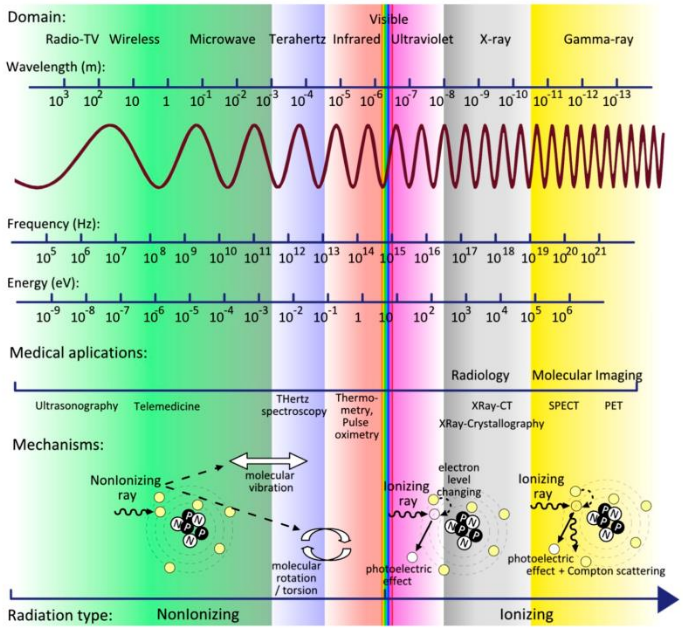


*Figure 1. The spectrum of electromagnetic waves, characteristics, and medical applications* [6]

***THz device***

In this project we will use the THz imaging and spectroscopy device "Terapulse 4000" produced by TeraView (Figure 2), composed of: integral unit for system control; optical system; electronic system equipped with integrated processors and external laptop that allows control and manipulation of the device, as well as data collection, processing and analysis.

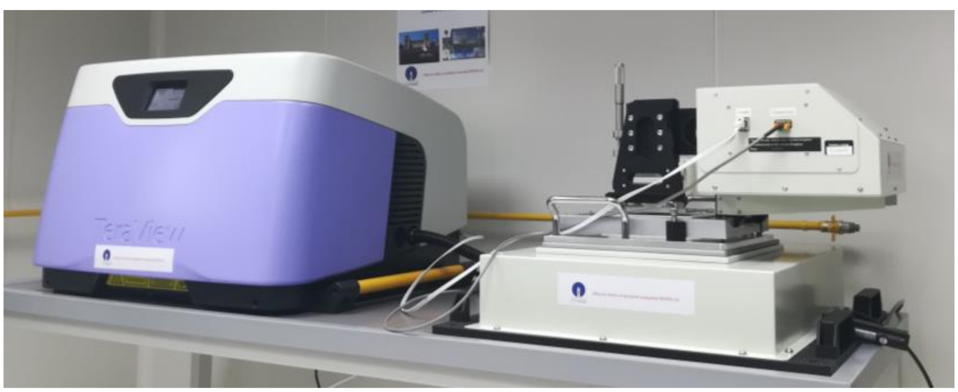

*Figure 2. Terapulse 4000 (TeraView)*

***Formulation and manufacture of samples, with technical recommendations***

In this phase, P1 has formulated 5 composite materials based on different mixtures of three raw materials and one reinforce. For the manufacturing of the materials has been first used a hot plate press, but this method proved to have some drawbacks. For this reason P1 has finally chosen to use a melt injection machine.

***Formulation and adaptation of the experimental model to TDTTS***

For excitation of molecules, a pulsed THz radiation (a femtosecond pulse laser) is applied and focused on the sample, transmitted, re-collimated and focused onto the THz detector. By moving a delay-line in the optical path of the laser beam, the time delay between excitation and detection of the THz pulse is varied, and the THz pulse is sampled in a time-resolved way. The THz spectrum is obtained by Fourier transform (FFT) of the time-resolved signal; from the phase and the amplitude information, the frequency-dependent THz material parameters (refractive index and absorption coefficient) can be directly obtained.

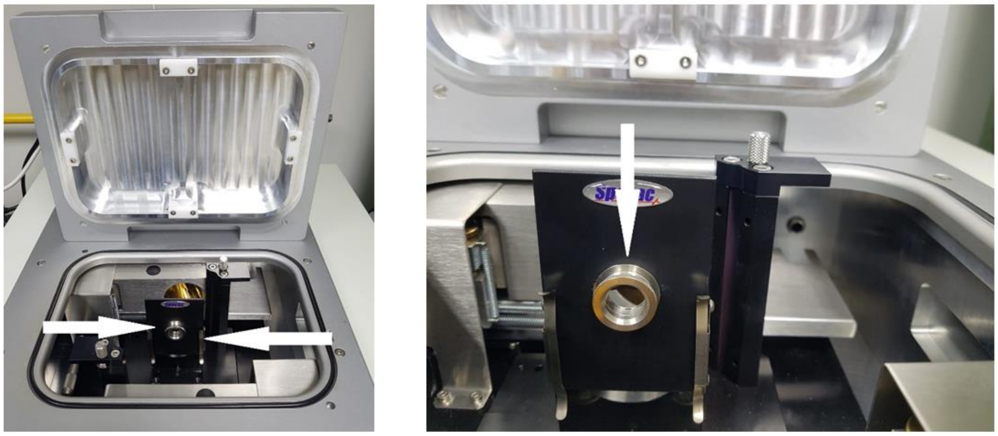

*Figure 3. TDTTS module*

***Conclusion***

The deliverables associated the objective of phase 1:

- *Design and experimental evaluation of TDTTS for composite materials obtained through recycling processes by the partner ALL GREEN SRL (CO);*
- *Formulation and adaptation of the experimental model to TDTTS (CO);*
- *Formulation and manufacture of samples, with technical recommendations (P1);*
- *One activity report.*

***References***


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