**CEFIC Long-range Research Initiative**

**Request for Proposals (RfP)**

***Title and Code Number:***

**Develop mechanistic model for fragmentation of microplastics in various environmental compartments – ECO59**

***Background***

There is increasing concern regarding the environmental fate and potential risks associated with microplastic particles, particularly with respect to their potential to degrade and fragment towards nano-sized particles. However, there is a lack of evidence of their presence or non-presence in the environment, due to the inadequacy of monitoring and analytical methods used to date. Furthermore, currently there is limited understanding regarding the potential of microplastic particles to degrade and fragment into nano-sized particles. Uncertainty with respect to occurrence, rate of formation, and the environmental fate continues to be used as a mechanism to speculate on the extent of potential risks.

The processes influencing fragmentation of micro- to nano-plastic and the rate at which this occurs represents a fundamental knowledge gap. Generally, the fragmentation of solid particles can be perceived as a common example of randomness and disorder, however, as demonstrated by ter Halle et al. (2016), with respect to the fragmentation of microplastic particles, it is possible to derive mathematical functions capable of estimating the fragment size/mass distribution. For instance, models based on the maximum-entropy method have been used to provide mechanistic insight of the fragmentation of a variety of processes such as in mining, the fragmentation of space debris and aerosol droplets (Englman, 1991). Results from ter Halle et al. (2016) suggest that the fragmentation of cubic-shaped particles, for instance, may result in greater potential to form smaller and smaller fragments then parallelepiped-shaped particles.

Due to their higher bioavailability potential, nano-sized particles may represent greater risks. Mathematical modelling approaches capable of estimating exposure will thus prove invaluable. Consequently, additional research that could strengthen mechanistic insight regarding the extent of fragmentation of plastic, which accounts for both the intrinsic physicochemical properties of the plastic and the extrinsic environmental factors, such as the UV, mechanical, chemical and biological degradation of the particles would be useful in helping guide monitoring activities as well as informing the potential for risk.

Mathematical modelling should be used to shape the design of experimental work that would illustrate the fragmentation to nanoparticles, or lack thereof, as there is a need to provide experimental evidence on the fate of Microplastic particles. This activity would utilize fundamental principles of thermodynamics in developing mathematical functions capable of estimating the fragmentation size distribution of plastic particles in the environment. The development of a mechanistic model to estimate the fragmentation size distribution of plastic particles in the environment would help to characterize and quantify environmental exposure to micro- and nano-plastic, as well as help guide future monitoring and risk assessment approaches.

***Objectives***

* It is proposed to develop a mechanistic model to describe the fragmentation size distribution of plastic particles in the environment for various types and shapes of plastic polymeric materials and under various relevant environmental conditions (water, air, soil and sediment).
	+ Model results should be validated with selected experimental fate testing with adequate analytical techniques.
	+ Source code developed should be easily transferable into environmental exposure models on microplastics
* If there is enough energy to thermodynamically fragment to nanosized materials, the model should also provide preliminary insights regarding aggregation/agglomeration potential for these nanosized fragments for potential future follow-up studies.
* As appropriate, experimentality derive a limited set of key default parameters (in a laboratory setting) if not readily available from literature.
* In developing the model, the adoption of the recommended six principles of “Good Modelling Practice” (GMP) should be followed (Buser et al, 2012). Notably, specify the input and output data entirely, conduct a sensitive analysis to identify the input parameters that have the greatest influence on the key results, and specify the limitations and limits of applicability of the model results.

***Scope***

* Fragmentation of microplastics
* Size distribution of fragmentation down to thermodynamic limits
* All types of synthetic solid plastic polymeric materials are in scope. The RfP is not restricted to certain type of microplastics e.g. polyolefin origin.
* Environmental conditions in aquatic, atmospheric, terrestrial and benthic systems.

***Deliverables***

* A mechanistic microplastics fragmentation model which has undergone validation.
* Publications in top tier peer-reviewed journals including full publication of the model. The computational model shall be provided open source including documentation.
* Presentations at scientific meetings to summarise results and obtain feedback on research directions.

The final report shall contain an executive summary (2 pages max), a main part (max. 50 pages) and a detailed bibliography. It is expected that the findings will be developed into at least one peer reviewed publication, following poster(s) and presentation(s) at suitable scientific conference(s).

***Cost and Timing***

Start in Q3 2021, duration 2 years

Budget in the order of €250K

***Partnering / Co-funding***

Applicants should provide an indication of additional partners and funding opportunities that can be appropriately leveraged as part of their proposal. Partners can include, but are not limited to industry, government/regulatory organizations, research institutes, etc. Statements from potential partners should be included in the proposal package.

***Fit with LRI objectives / Possible regulatory and policy impact involvements / Dissemination***

Applicants should provide information on the fit of their proposal with LRI objectives and an indication on how and where they could play a role in the regulatory and policy areas. Dissemination plans should also be laid down.

***References***

* Englman R. 1991. Fragments of matter from a maximum-entropy viewpoint. Journal of Physics: Condensed Matter 3(9): 1019-1053.
* Ter Halle A, Ladirat L, Gendre X, Goudouneche D, Pusineri C, Routaboul C, Tenailleau C, Duployer B, Perez E. 2016. Understanding the fragmentation pattern of marine plastic debris. Environ Sci Technol 50(11): 5668-5675.
* Buser AM, MacLeod M, Scheringer M, Mackay D, Bonnell M, Russell MH, DePinto JV, Hungerbuhler K. 2012. Good modelling practice guidelines for applying multimedia models in chemical assessments. Integrated Environmental Assessment and Management. 8(4): 709-708

**DEADLINE FOR SUBMISSIONS: June 30th, 2021**

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