

Going "FAIR" Experiences from NanoFASE – NanoCommons TA

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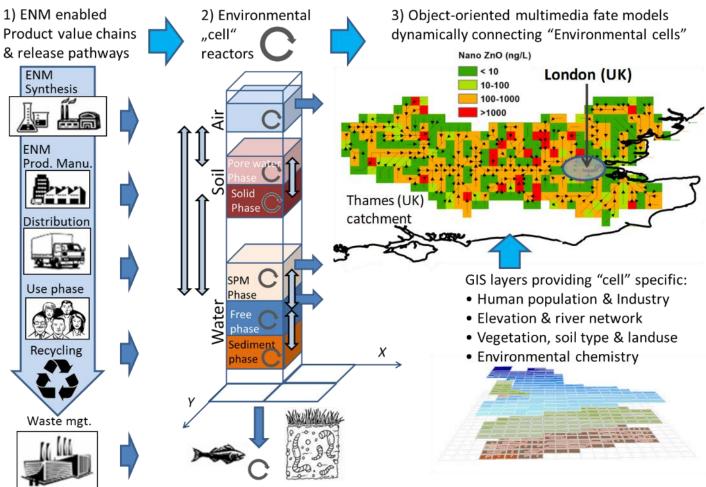
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Christine Hendren, Mark Wiesner - Duke





How much is released, and where does what go?

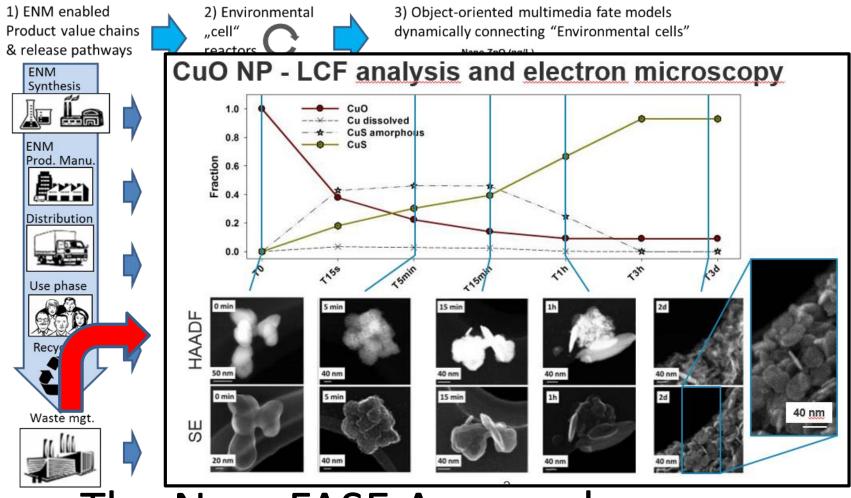


The NanoFASE Approach





How much is released, and where does what go?

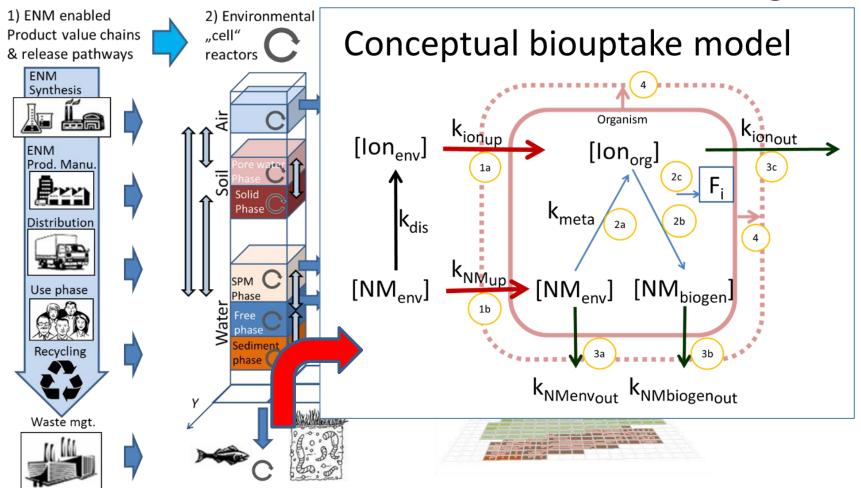








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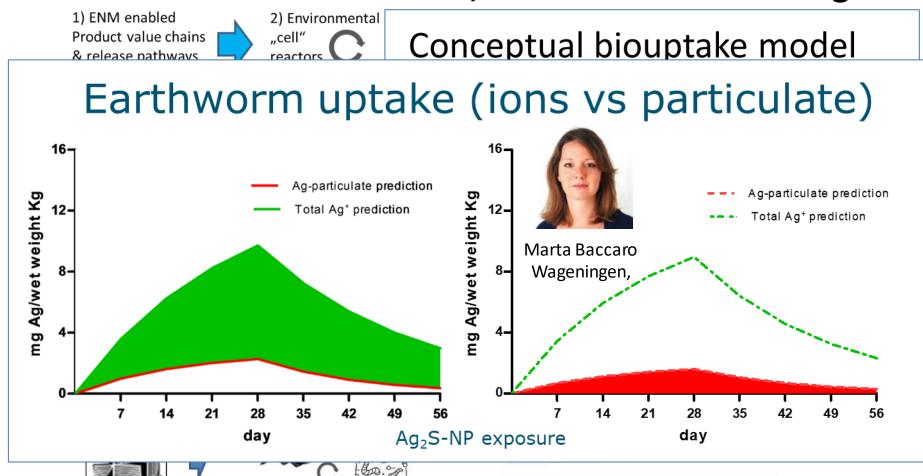


The NanoFASE Approach





How much is released, and where does what go?









Exposure - Nanomaterial fate in the environment:

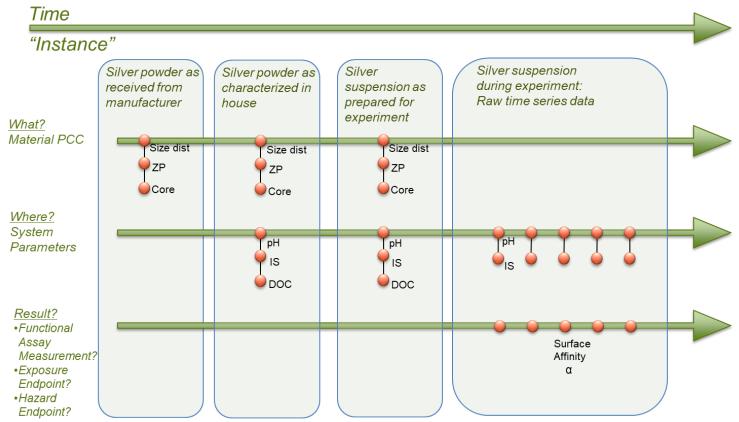
How did we plan to handle, share and store the data?

On the NIKC Concept of "Instance"
Temporally and Spatially Tracking the Path of a Study







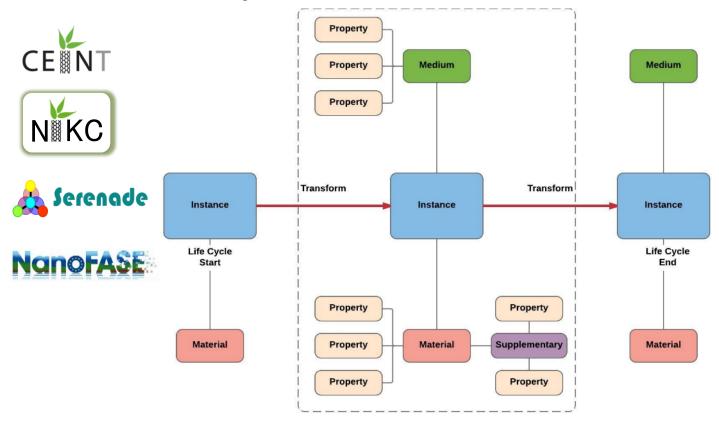






Exposure - Nanomaterial fate in the environment:

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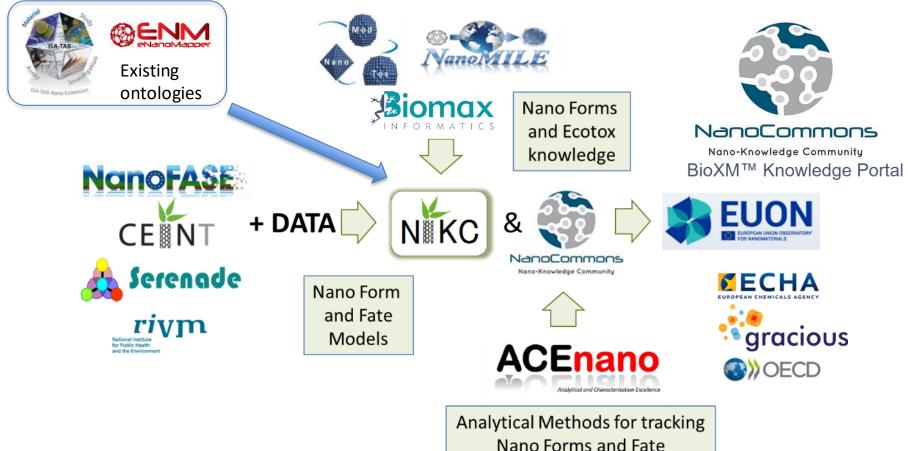






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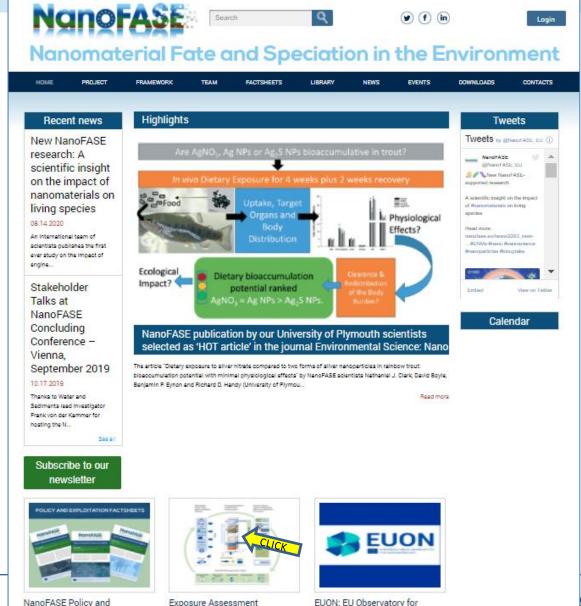
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NanoFASE "Clickable Framework" modules



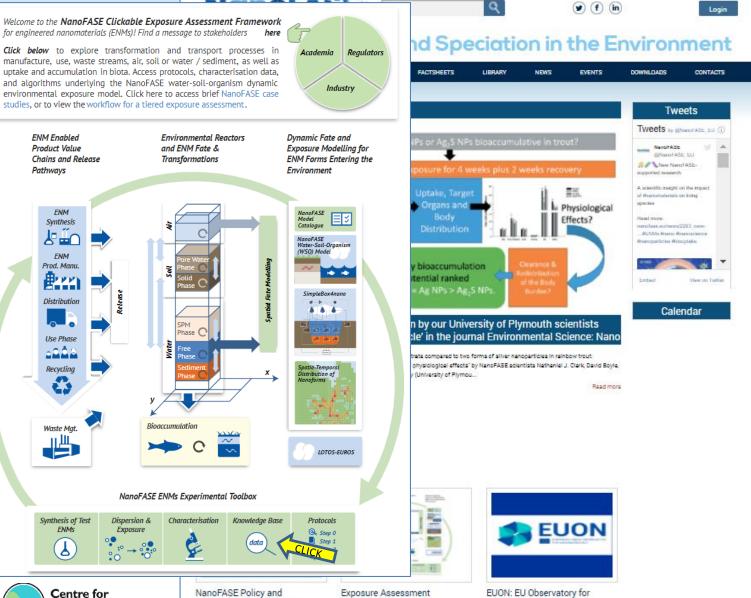
Nanomaterials



Exploitation Factsheets

Framework

NanoFASE "Clickable Framework" modules





Framework

Exploitation Factsheets

Ecology & Hydrology

NATURAL ENVIRONMENT RESEARCH COUNCIL







NanoFASE Exposure Assessment Framework

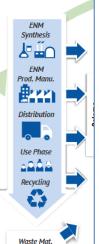
Welcome to the NanoFASE Clickable Exposure Assessment Framework

Click below to explore tran manufacture, use, waste strear uptake and accumulation in bic and algorithms underlying the environmental exposure mode

studies, or to view the workflow

for engineered nanomaterials (EN

ENM Enabled Product Value Chains and Release Pathways



NanoFASE ENMs Experimental Toolbox



In order to be able to predict the behaviour of engineered nanomaterials (ENMs) in the environment, NanoFASE proposes a catalogue of environmental fate models. The model parameters are derived from experimental work relying in turn on sets of test ENMs synthesized specifically for the project, or acquired from industry partners or commercial suppliers. The ENMs used for NanoFASE provide very specific features to facilitate the conduct and interpretation of the experimental work, for example: labelling to track test ENMs against a high background of similar particles occurring naturally; test particles such as silver sulfide ENMs mimicking the transformations that ENMs undergo when released to the environment.

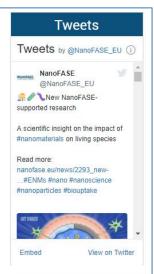
All NanoFASE ENMs were extensively characterised under the exposure conditions relevant for the measurement of ENM fate and behaviour as they move through the environmental 'reactors' of <u>air</u>, <u>water and sediment</u>, <u>soil</u>, and/or <u>waste water treatment plants</u> (<u>WWTPs</u>) and in the relevant <u>biota</u>. In the Clickable Framework, visitors can access detailed descriptions of procedures for dispersion and for characterisation, with links to existing (e.g. OECD) procedures, or to newly developed NanoFASE procedures including Functional Fate Assays to determine specific model parameters, such as attachment efficiency in soils.

Finally, all of the data generated within NanoFASE is captured in the NanoFASE Knowledge Base, linked to the relevant procedures, ontological terms, ENM characterisation, and relevant case studies, allowing intelligent searching of the data and development of predictive models.

Click on each of the images below for more details of these tools.

NanoFASE ENMs Experimental Toolbox





Calendar



Synthesis of Test ENMs



NanoFASE Exposure Assessment Framework



Click below to explore tran manufacture, use, waste strear uptake and accumulation in bid and algorithms underlying the environmental exposure mode studies, or to view the workflow

> **ENM Enabled** Product Value Chains and Release **Pathways**



Knowledge Base



At term the extensive experimental data collected and structured by NanoFASE will be rendered FAIR: Findable. Accessible, Interoperable, and Re-usable, across Europe and beyond. This implies both project-based efforts and participation in European or EU-US Communities of Research joint initiatives, such as EUON or the CEINT NanoInformatics Knowledge Commons (NIKC).

Learn about NanoFASE contributions to European nanosafety harmonisation and the European Union Observatory on Nanomaterials (EUON).

The NanoFASE knowledge base embraces metadata, ontology and terminology, as well as experimental protocols and procedures.

Metadata

NanoFASE uses the Biomax platform for project traceability, managing nanomaterials stock, orders and data. The project used industry-produced nanomaterials for realism, and bespoke synthesized particles suitable for more controlled experiments. All the studies undertaken across the empirical work packages produce data to parameterise the NanoFASE fate and exposure models. Partners used the NanoFASE-tailored Biomax platform to order the nanomaterials needed for their experiments. Material Safety Data Sheets, shipping and characterization data are all present in our Biomax portal for download. Templates were generated for data capture to facilitate the upload and preservation of all experimental data.

Through this centralized platform all NanoFASE partners are aware of which NMs are being used in which experiments across the consortium. University of Birmingham collaborated with the empirical work packages to enlarge the characterization templates, assembling descriptions and state-of-the-art images of pristine particles, as well as the protocols for how the data was generated. Together, these are intended to provide a resource capturing the great diversity of distinct information produced by our complex multimedia studies and to feed the modelling tools.

Ontology and terminology

Finally NanoFASE's interdisciplinary approach to the science behind understanding the environmental fate of engineered nanomaterials highlights the need for meta-level integration of terminology and data. Technical words may have multiple meanings and a lack of harmonisation between scientific disciplines or even between projects can hinder the transfer of ideas between fields and potentially limit the efficient linkage and enhancement of Click of data and knowledge. This issue has been addressed by e.g. eNanoMapper and the Bioportal by building a shared ontology of relevant terms. The NanoFASE Clickable Framework itself contextualizes important terms and concepts, improving access by making them easily searchable and crossreferenced throughout the website.

Up to now such ontological efforts within nano environment/health/safety research have mainly focused on the toxicological and material sciences fields. NanoFASE has worked closely with the US Center for the Environmental Implications of NanoTechnology (CEINT) to build the extra terminology for referencing the different issues and processes relevant to the environmental fate and transformation science we have done. This work will provide an exemplar and a template for the terminology used in future nano projects dealing with environmental fate and uptake.

Data capture templates

NanoFASE has cooperated closely with the CEINT NanoInformatics Knowledge Commons (NIKC) initiative. The NIKC is a custom cyberinfrastructure consisting of a data repository and associated analytical tools developed to visualize and interrogate integrated datasets. NanoFASE and other NanoSafety Cluster projects have demonstrated the capacity for global data entry to NIKC, expanded to include exposure related studies, and specifically exposure across the nano-enabled product value chain.



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Calendar



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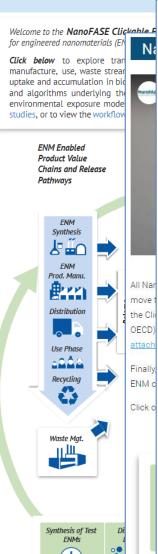






Synthesis of Test FNMS

NanoFASE Exposure Assessment Framework



Knowledge Base

Knowledge Base

data

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Data capture templates

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NanoFASE mesocosm-generated datasets were deposited into the NIKC as a pilot project with a view to expanding these efforts to other studies carried out as part of NanoFASE. The efforts were accelerated through the development of data templates and curation of datasets in collaboration with the NanoCommons project, as well as several training seminars for NanoFASE researchers on data entry, led by CEINT (Duke University) and University of Birmingham. NanoFASE is working to ensure that this part of its legacy remains available to the field in the future, by collaborating closely with the NanoCommons e-infrastructure.

The data capture template used by NanoFASE is presented* with instructions in the form of two tutorials. One is a <u>visual/graphical manual</u>, and the second is a <u>text-based manual</u> the contains all the analytical details of the process. The template and manuals were produced in a close <u>CLICK</u> transatlantic collaboration with Currellock ke University and drafted by Team Helium. The Summer 2019 version of each tutorial may be updated and refined going forward and will be uploaded to the NanoSafety Cluster website. The template and tutorials are intended to serve the entire nano environmental health and safety community worldwide.

Contact



Anastasios (Tassos) Papadiamantis

University of Birmingham

NanoFASE Exposure Assessment Framework lected and structured by NanoFASE will be rendered FAIR: Findable, **Tweets** ross Europe and beyond. This implies both project-based efforts and nities of Research joint initiatives, such as <u>EUON</u> or the CEINT Tweets by @NanoFASE_EU (i) The NanoFASE NIKC Curation Manual EINT NanoInformatics Knowledge Commons (NIKC) initiative. The NIKC is a custom cyberinfrastructure NanoFASE NIKC Curation Process ation 2 3 hd **Initiating Steps** NanoFASE I NIKC Correct any Fill NanoFASE Review curation Generate Customize **Curation Manual** errors in NanoFASE Excel **Excel Template** manual and instance Shared dataset and **Template** with Dataset(s) note any map as a Curator Meeting send to visual (columns, questions the Schedule Set curator abstract* parameters) ~1.5 hours ~2 hours ~4-5 hours* ~24 hours * Review with Review with Review with Review with curator to curator to curator to curator to resolution. resolution. resolution. resolution. ~0.5 hour Curator ~1 hour ~2 hours ~16 hours **UPLOAD** *Depends on size of dataset * This step may be moved to the end if the data owner prefers to work in the Excel template first **NanoFAS** NIKC NanoFA consistil

UK Centre for Ecology & Hydrology



Nanomaterial fate in the environment – Methods and **Data delivered**







www.NanoFASE.eu (EU H2020 Proj. 646002)









