# Computational assessment of the environmental transport and fate of small molecules and PFAS using the SimpleBox4Planet web-application

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## 1. Introduction

Per- and polyfluoroalkyl substances (PFAS) are present in a wide variety of industrial processes and consumer products. Nonetheless, they are increasingly being identified as environmental pollutants, and some have been associated with adverse effects on human health. Their structure includes carbon-fluorine bonds, which are among the strongest chemical bonds; thus, they are resistant to degradation both during use and upon release to the environment ("forever chemicals"). In fact, PFAS are regularly found to contaminate groundwater, surface water, and soil[1–3]. In this scope, the PROPLANET project supports the development of safe and sustainable by design (SSbD) coatings that will substitute the PFAS-type coatings used in the textile, food packaging and glass industrial sectors[4]. To support the SSbD principles, the PFAS alternative substances are explored *in silico* to assess their environmental transport and fate. A customized SimpleBox[5] model, incorporating the specific properties of the PROPLANET candidate PFAS alternative substances, is used to simulate their concentration in air, water, sediment, and soil. The produced results can be later supporting the assessment of potential risks throughout the coatings' lifecycle. To ensure the use of the SimpleBox model from the wider community (including industry and regulators) the Excel version of the model is incorporated into the SimpleBox4Planet tool where all the necessary input parameters are streamlined in a user-friendly interface. The SimpleBox4Planet tool is also available through Application Programming Interfaces (APIs) for integration with the PROPLANET Replication tool enabling simulation of coating behaviour under various conditions and supporting SSbD.

## 2. Development of the SimpleBox4Planet tool

The SimpleBox[6] is a nested multimedia mass balance model that simulates the transport of chemical substances between different homogeneous environmental compartments (e.g., air, water, soil, etc.) in different landscape settings, developed as an MS Excel® spreadsheet. The SimpleBox4Planet tool provides a user-friendly environment (Figure 1, https://www.enaloscloud.novamechanics.com/proplanet/simplebox4planet/) without compromising the capabilities of the original SimpleBox Excel-based version. Furthermore, the SimpleBox4Planet is available through APIs (https://www.enaloscloud.novamechanics.com/proplanet/swagger-ui/) so that it can be easily integrated into the PROPLANET Replication tool. The user can select the

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substance of interest from the available list of PFAS alternatives and one of the available exposure scenarios and calculate the environmental fate of the substances (mass flows between air, water, sediment, and soil) on regional, continental, and global spatial scales.

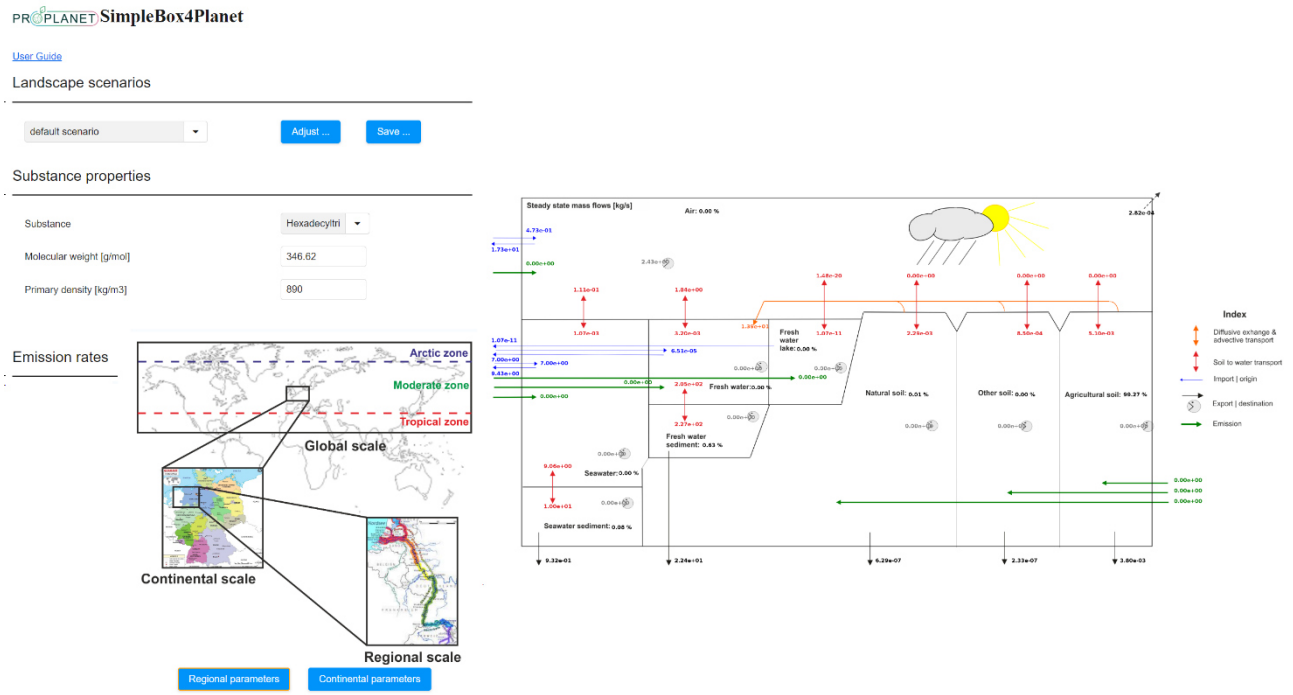


*Figure 1: Screenshot of the SimpleBox4Planet tool input and output.*

The candidate PFAS alternatives assessed under the PROPLANET project and incorporated into the SimpleBox4Planet tool are:

- Acetic acid,
- Hexadecyltrimethoxysilane,
- Octyltrimethoxysilane,
- Hexamethyldisiloxane,
- Methyltrimethoxysilane,
- Trimethoxyphenylsilane,
- 2-Octenylsuccinic anhydride,
- Dodecyltriethoxysilane,
- Polysiloxanes, di-Me, hydroxy-terminated,
- Polysiloxanes, di-Me (Silicon oil),
- Starch (Corn starch),
- Zinc oxide (ZnO),
- Sodium alginate,
- Chitosan,
- Glycerol,
- 2-Oxetanone, 3-C12-16-alkyl-4-C13-17-alkylidene derivs. (AKD).

The SimpleBox4Planet tool includes an updated database with the properties of the candidate PFAS alternative compounds collected through an extensive database search in PubChem database (https://pubchem.ncbi.nlm.nih.gov/), CAS registry (https://commonchemistry.cas.org/), the ECHA Chem (https://chem.echa.europa.eu/) registration dossiers and the substances safety data sheets. To fill the potential data-gaps, properties were estimated using in-house Quantitative Structure-Property Relationship (QSPR) models for the prediction of the substances' water solubility, vapour

pressure and octanol/water partition coefficient. To use these models, the substance's structure is only needed as input (e.g., in SMILES or SDF format), and the necessary molecular descriptors are automatically calculated using the Mold2[7] software. For comparison purposes three PFAS substances are also included in the SimpleBox4Planet tool; the Perfluorobutanoic acid (PFBA), the Perfluoropentanoic acid (PFPeA), and the Perfluorobutane sulfonic acid (PFBS). Their relevant properties were extracted from the Interstate Technology and Regulatory Council (ITRC) online documents (https://pfas-1.itrcweb.org/).

## 3. Conclusions

The ability to predict the exposure of chemicals including PFAS in the environment is crucial in assessing their potential risks. However, conducting exposure assessments for chemicals can be expensive and time-consuming, especially when dealing with large numbers of substances. Screening level environmental exposure models such as the SimpleBox model, provide a cost-effective and efficient solution to this problem, as they are designed to provide conservative estimates of exposure without the need for complex data requirements, making them a valuable tool in regulatory environmental risk assessment. However, the stakeholders, including industry professionals, regulators, and consultants, are not typically experts in modelling or software development. Therefore, it is essential that these screening level exposure models have intuitive and user-friendly interfaces. To address this issue, the SimpleBox4Planet web-tool based on the SimpleBox Excel version was developed. It is also available through APIs, making it accessible to anyone interested in using it directly or integrating its functionality into their own software. The development of user-friendly screening level exposure models is a critical step in facilitating the responsible use and regulation of PFAS and other chemicals, helping to ensure their safety and minimize their potential risks to the environment and human health.

## 4. References

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