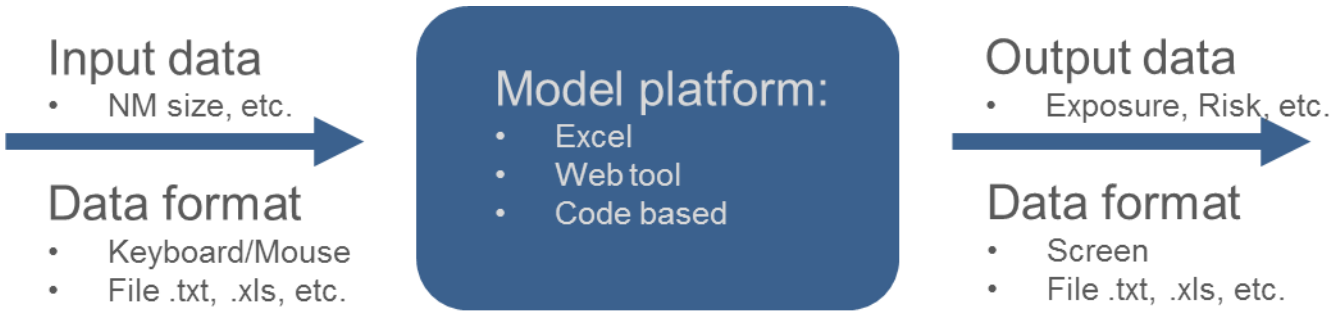
caLIBRAte
nano risk governance

Fact Sheet

Input requirements and data formats of Nanomaterials risk assessment tools

One goal of the caLIBRAte project was to test the sensitivity and performance of Nanomaterial (NM) risk, exposure and hazard assessment models. To carry out this task and to implement a feasible and efficient methodological testing approach, information was needed on model input requirements along with data formats. This included technical information on 20 models identified in early stage of the caLIBRAte project. Generation of such information was the first step on the road to implementing the sensitivity testing and data gap analysis in caLIBRAte.



Input data is defined as values that the model users are required to provide to the computational system in order for the model to perform its task and to obtain the output value.

Input data requirements

- The analysis of the input data revealed that the majority of inputs required of the models were very heterogeneous, and overlaps were not in the majority.
- For the 20 models, a total of 1190 different input parameters were identified. This includes 16 nanospecific models for which 990 input parameters were identified. Of these, only a small subset is shared between different models.
- Some examples of shared input parameters include particle size, particle density, temperature, particle attachment efficiency, emission rate, solubility, fraction of the NM in the substance, dustiness, room dimensions, ventilation rate, duration of process, hazard statements and limit values.
- These shared variables of different models will be critical for comparisons between the models, as they represent an opportunity for direct model inter-comparison with the same input.
- This work resulted in a thorough documentation of the input and output parameters space of the models and tools used in nanomaterial risk assessment

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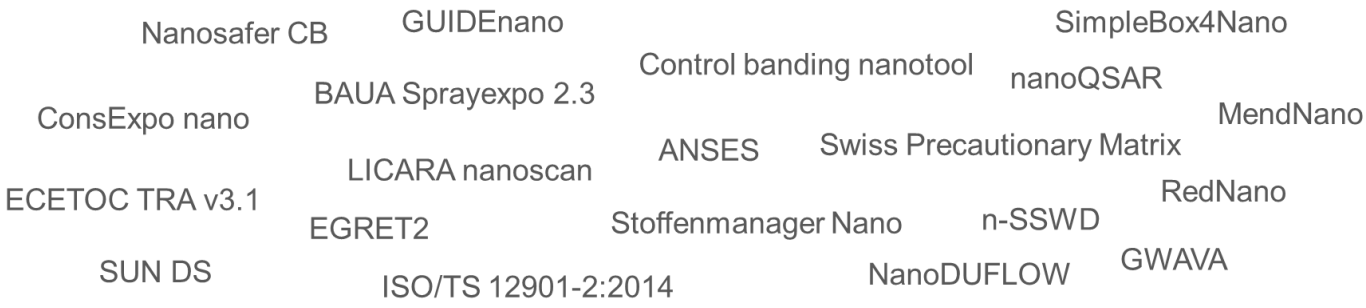
Model platforms and data formats

The predominant platforms for model implementations are Excel sheets (8/20) and web interfaces (8/20). Other including simulation package (Duflow), programming languages (Fortran, Python) or not being implemented as a software. User interfaces are therefore predominantly implemented using Excel and Web applications, sometimes with a graphical user interface available. Following this, the input data formats also vary between the models. Six models require direct user input via mouse and keyboard, and the use of pre-determined input files is not prevalent. Five of the tools have the possibility of using a prepared input file using Excel and six of the models either allow or need a text, xml or csv-file as an input. For one of the models it is indicated that a combination of ASCII and binary files is used. Output data is mostly (10/20) acquired directly from the program screen when the model is used. Output file generation is possible for 10/20 models, either in Excel, text, csv, pdf, h5 or xml- file formats.



Consequences for model testing

The data formats used in the models were found to be relatively simple. More than half of the models are implemented in Excel and use Excel files as input or output. Other half is either web based or implemented some other way. Therefore, automatized testing systems are needed for Excel and Web based tools to effectively test their sensitivity and performance.

In general, no principal difficulties in transferring data to the models were identified. No proprietary data formats were used, and the inputs have low complexity. However, it should be noted that the input requirements for the models are extensive, which introduces a challenge for the data generation. Therefore, a prioritization of input parameters might be necessary.

This fact sheet is based on caLIBRAte Deliverable 7.1: *Report on mapping of input requirements and data formats for the tools* produced as a result of collaboration between Tampere University (FI), National Research Centre for the Working Environment (DK), the Netherlands Organisation for applied scientific research (NL), National Institute for Public Health and the Environment (NL) and GreenDecision (IT).

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