Predicting the Fate and Transport of Insensitive High Explosive Constituents in the Environment

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Challenge posed by Insensitive High Explosives (IHE)

- IHE are explosives less sensitive to accidentally explode under non controlled detonations.
- IHE have unique physical, chemical and biochemical properties making them mobile and labile molecules in the environment.
- IHE have the potential to migrate through subsurface soil and to undergo (bio)transformation to other chemicals
- However, little is still known about their behaviour, toxicity and persistence in the environment.

What is the real impact of these chemicals on the environment?
How can they be assessed?

Need to investigate their transport and transformation mechanisms under genuine environmental conditions

Investigating into IHE transport – experimental methods

- It is not always straight forward to determine the pathways of real contamination in the field (air, land and water)
- We need to undertake experiments to understand explosive behaviour → predict where it goes (transport) and what happens to it (fate)
- It allows us to easily obtain results quickly
- The residues can be treated without contaminating the environment.
- Examples:
    - microcosms
    - bottle flask experiments
    - Soil columns

Predicting environmental behaviour: laboratory vs computers pros and cons

EXPERIMENTAL METHODS

- Time consuming → long periods to perform experiments
- Expensive cost → reagents, equipment, material…
- Not always replicable → e.g. soils change over time
- Site specific conditions → soils are unique
- Small scale

What can we use to support and help laboratory methods to be more representative of the real environment?

COMPUTATIONAL MODELLING

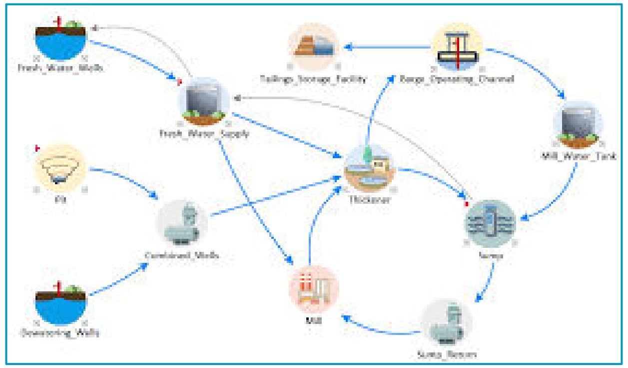
Computational programs

- Several computational programs have been developed to predict the fate and the transport of contaminants in the environment, but only few have been used specifically for explosives.

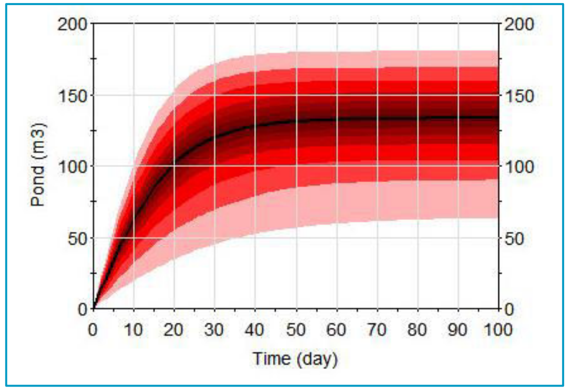
- HYDRUS is one of the most often reported for explosive fate and transport studies. However, it does not allow probabilistic simulations.

- Conversely, **Goldsim**

  1. **Multidisciplinary** → complex interactions
  2. **Representation of uncertainties** → decision making
  3. **User friendly**



A model that cannot be easily understood is a model that will not be used

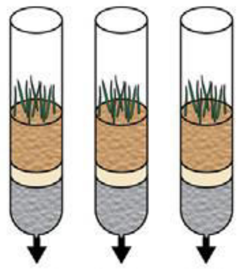


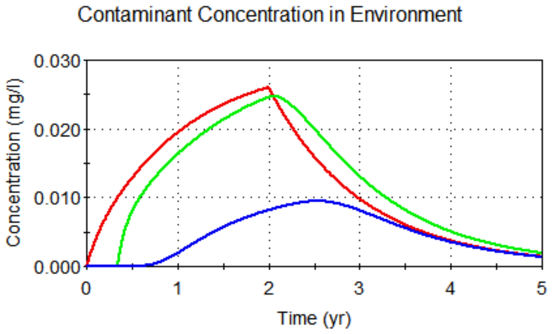
Aim

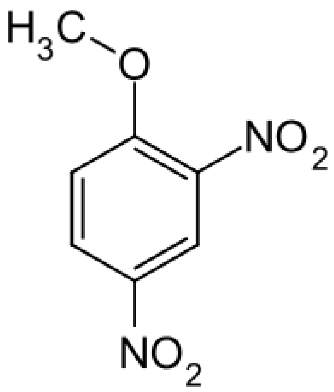
To simulate the transport of the IHE constituents DNAN and NTO in quartz sand columns using GoldSim by comparing breakthrough times and concentrations to laboratory experiments.

SOIL COLUMNS

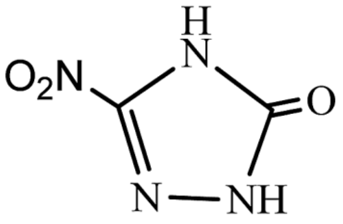
GOLDSIM







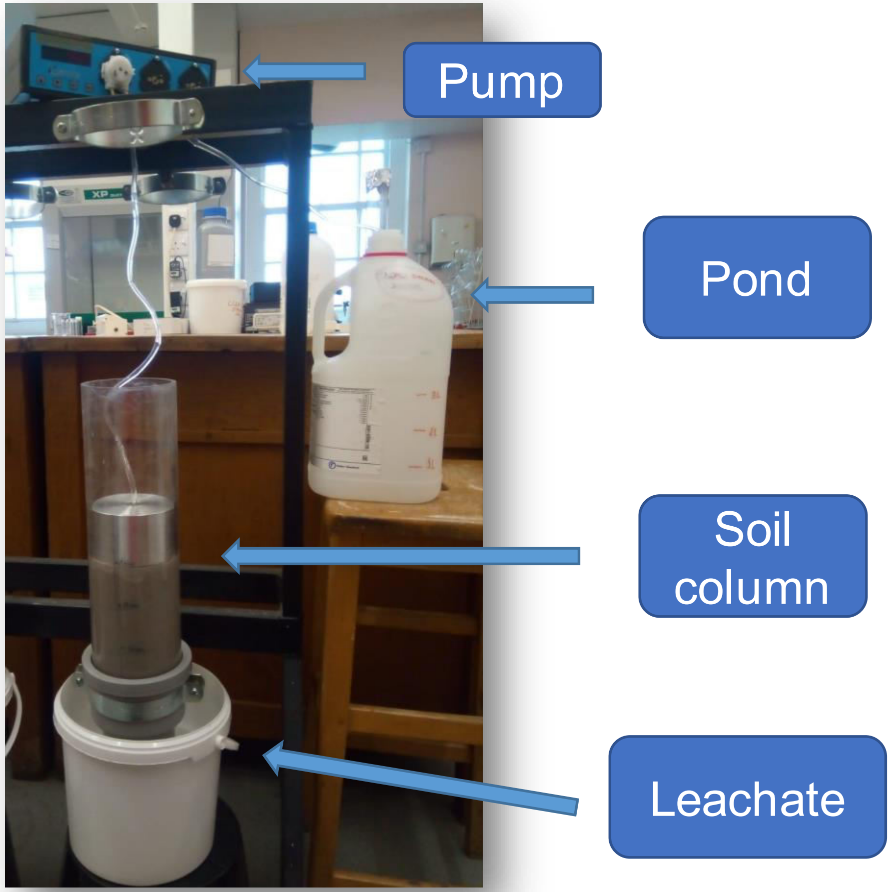
2,4- dinitroanisole (DNAN)



3-nitro-1,2,4-triazol-5-one (NTO)

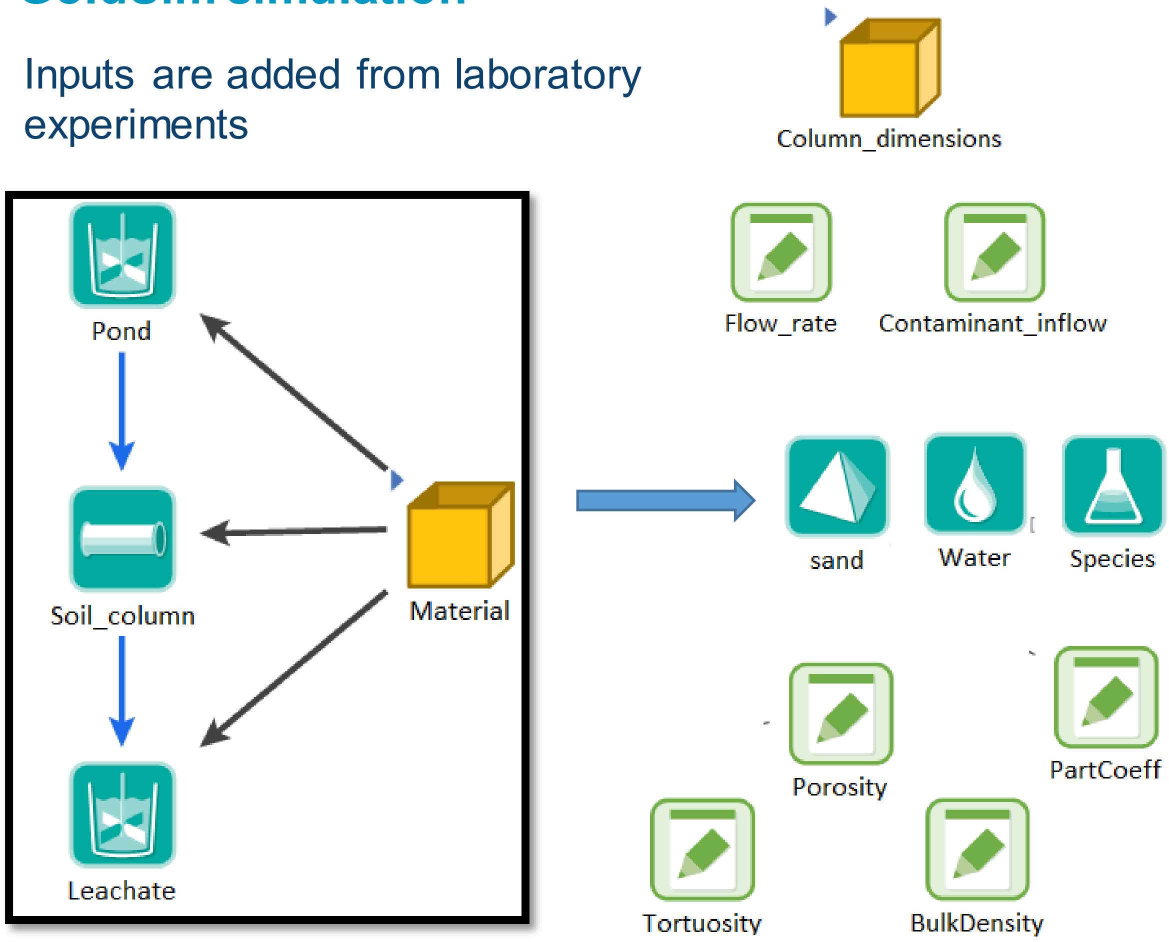
Methodology

Laboratory experiment

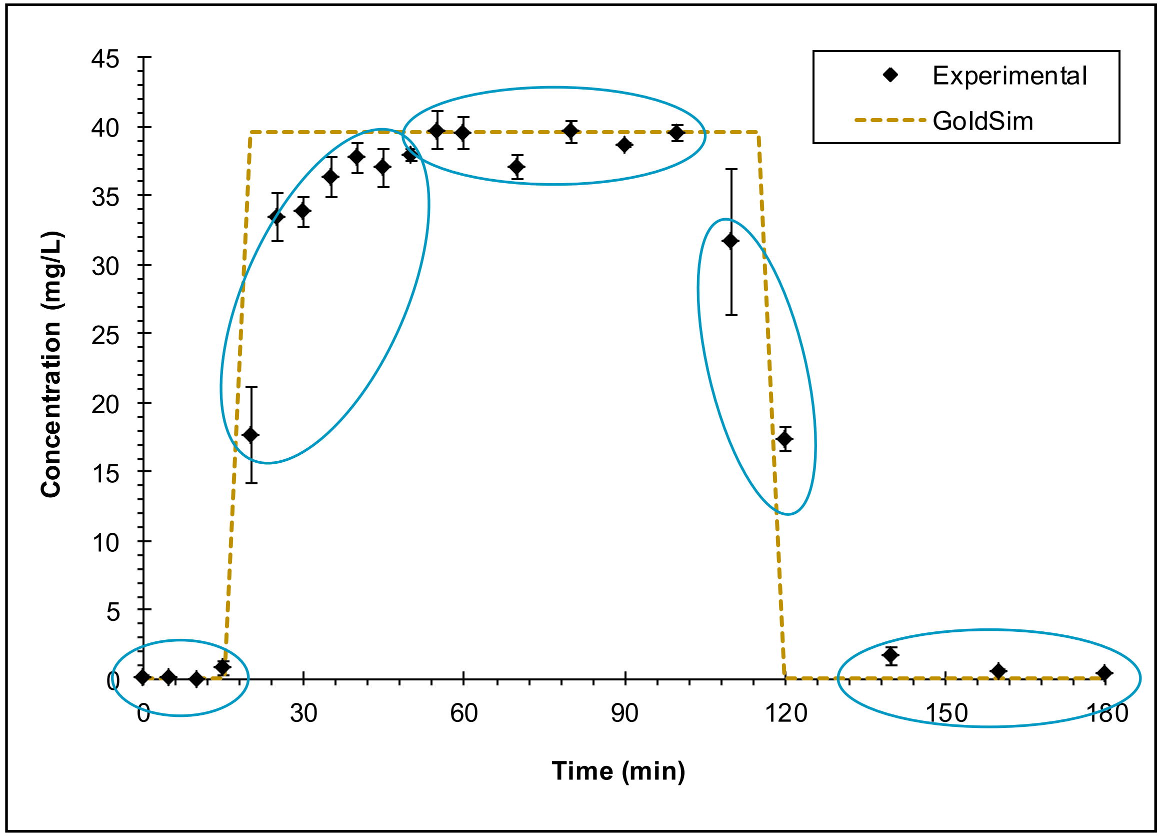


GoldSim simulation

Inputs are added from laboratory experiments

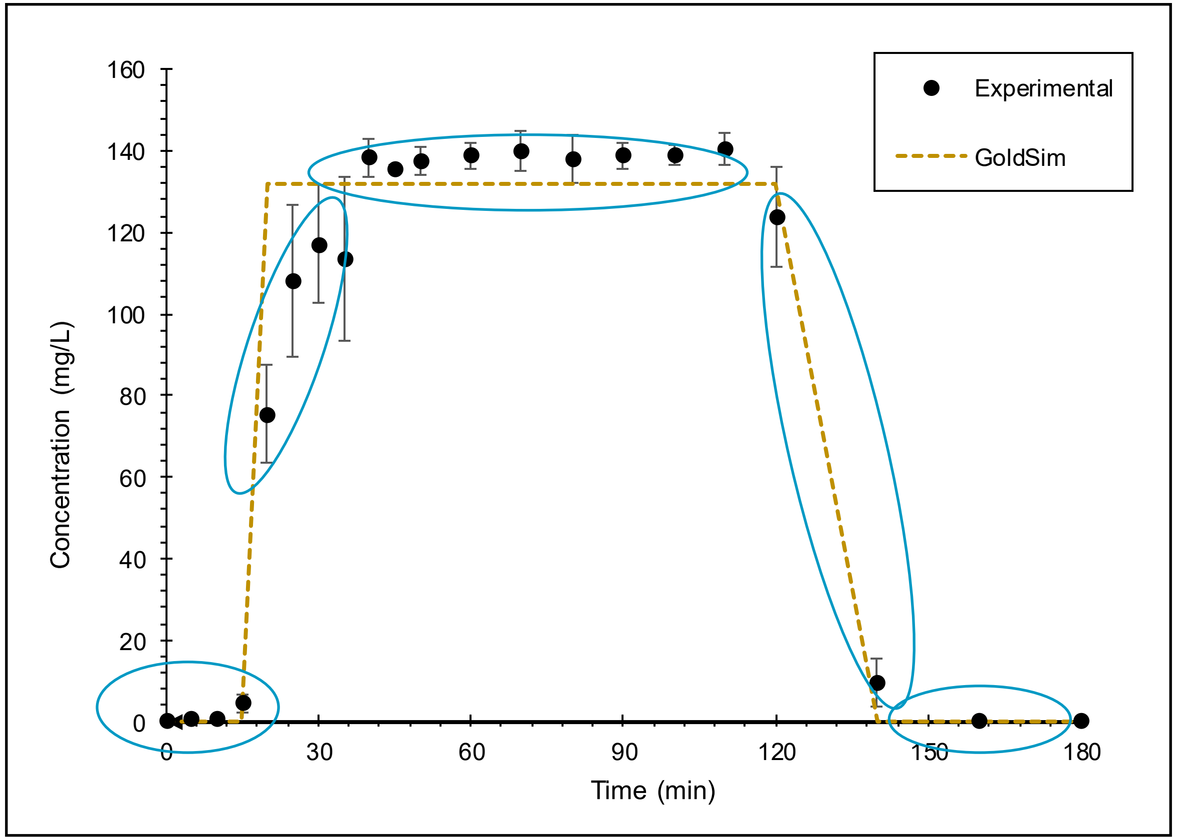


Results – DNAN breakthrough



- From 0 to 15 min → NTO only travels through the quartz sand
- From 15 to 45 minutes → experimental concentrations are lower than expected by GoldSim → retention?
- From 50 to 100 minutes → maximum concentrations, very similar to those predicted by GoldSim
- From 110 to 120 minutes → decrease of NTO concentrations.
- From 120 to 180 minutes→ practically no NTO.

Results - NTO breakthrough in the soil column

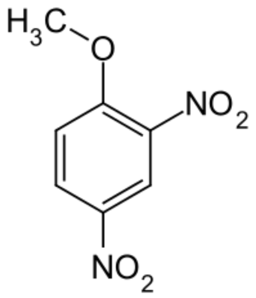


- From 0 to 15 min → no NTO came out of the sand column
- From 15 to 35 minutes → experimental concentrations are lower than expected by GoldSim.
- From 40 to 110 minutes → maximum concentrations, slightly higher than predicted by GoldSim
- From 120 to 140 minutes → rapid decrease of NTO concentrations.
- From 140 to 180 minutes→ practically no NTO.

Results - Recoveries

DNAN

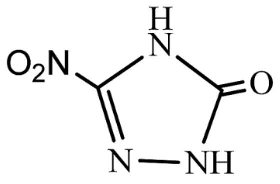
Approach	Recovery (%)
Experimental	93.3 ± 1.9
GoldSim	99.6 ± 1.5



- Almost all DNAN was recovered from the leachate of the quartz sand column
- Results are quite similar between simulation and experiment
- Experimental recovery is lower due to mass loss during the experiment

NTO

Approach	Recovery (%)
Experimental	101.37 ± 0.90
GoldSim	98.05 ± 0.13



- Results are quite similar between simulation and experiment
- NTO is very soluble → almost fully recovered
- Experimental results over 100% → systematic errors due to the procedure

Conclusions

1. This work confirms that GoldSim can be used to simulate the transport of IHE in quartz sand.

2. Contributed to understanding the transport of DNAN and NTO in a simple matrix with low organic content and few matrix-compound interactions.

3. Soil columns are an optimum experimental method to study transport of contaminants in the laboratory and also to use for comparing empirical results with computational simulations in GoldSim.

4. To better simulate transport in GoldSim, inputs (e.g. bulk density) must be derived from empirical data to ensure representativeness of real scenarios.

5. GoldSim simulations need further development to determine whether GoldSim is able to simulate mixtures of explosive compounds in more complex soils.

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