



Predicting the Transport of Insensitive High Explosive Constituents in Quartz Sand

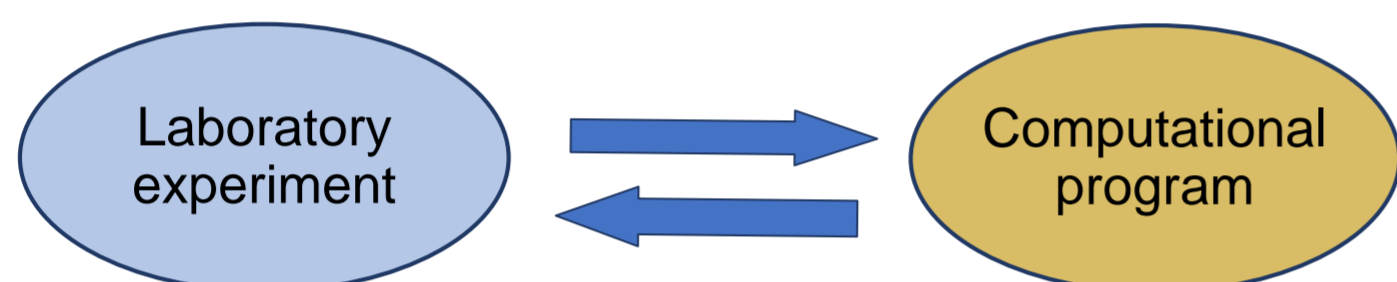
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Introduction and Aim

Investigating the environmental impact of explosives is challenging in the real environment as it is not possible to conduct controlled experiments or intentionally contaminate land. In addition, little is known about their toxicity and persistence, which raises the question:

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

The transport of two Insensitive High Explosive compounds, DNAN and NTO was experimentally investigated using quartz sand columns. Additionally, computational simulations were performed simultaneously to:



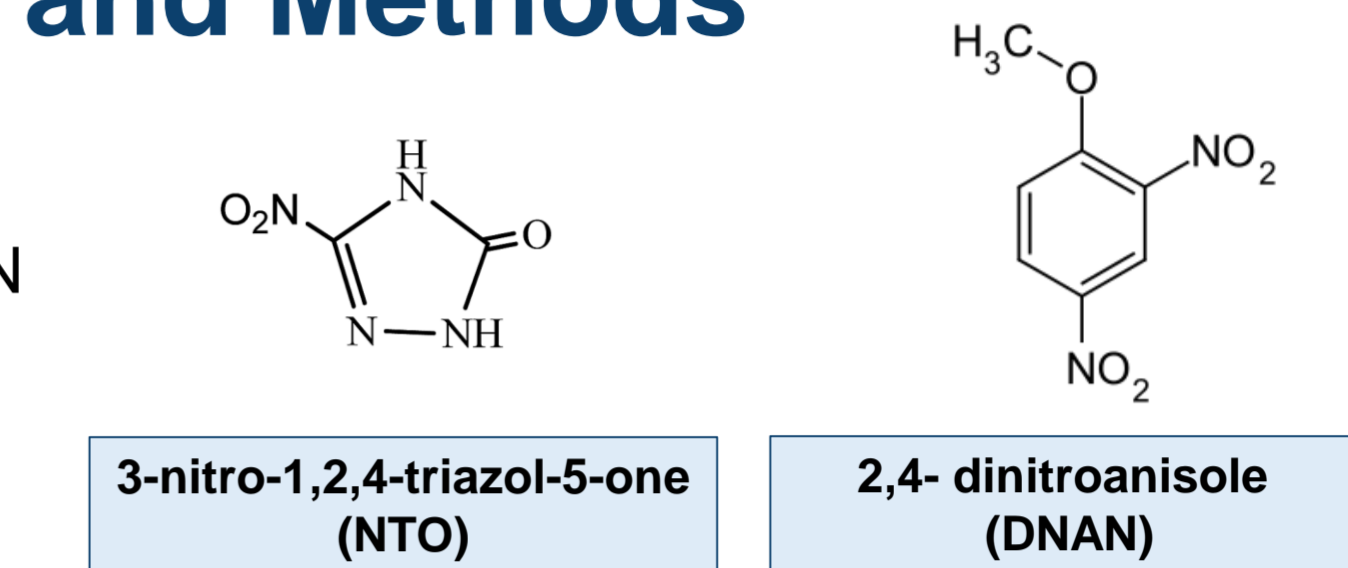
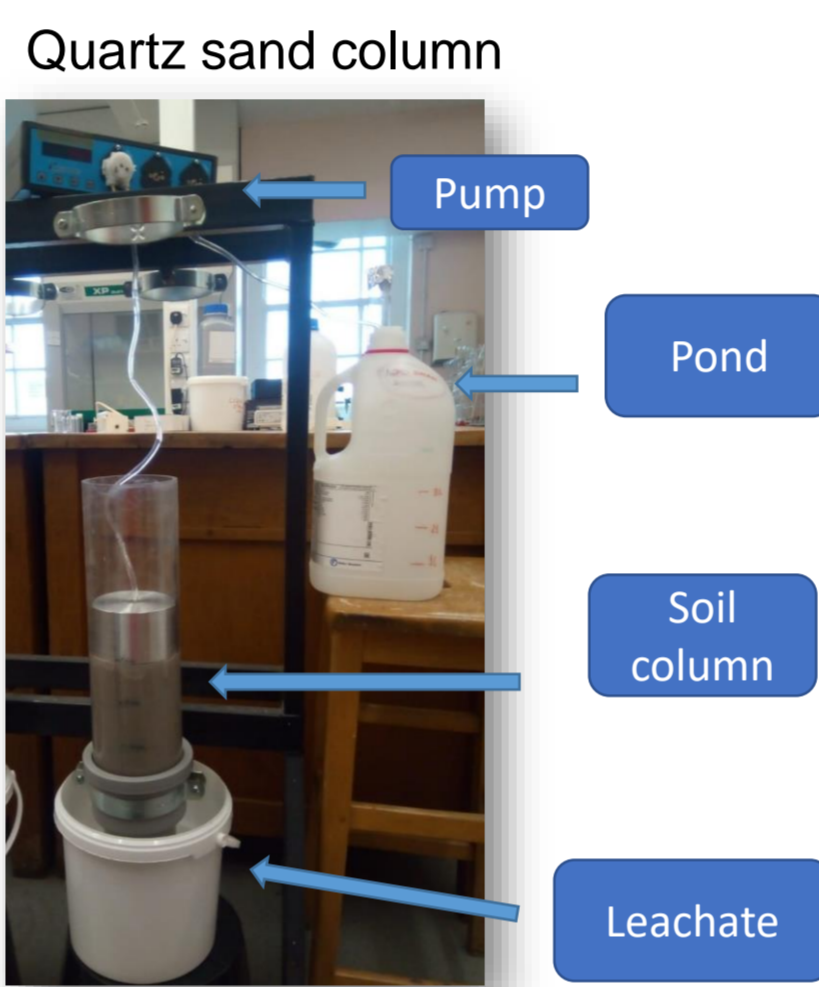
- Assess the extent to which Goldsim simulations can help to refine the prediction of IHE compounds in the environment
- Determine whether GoldSim can be a representative alternative to laboratory experiments.

Material and Methods

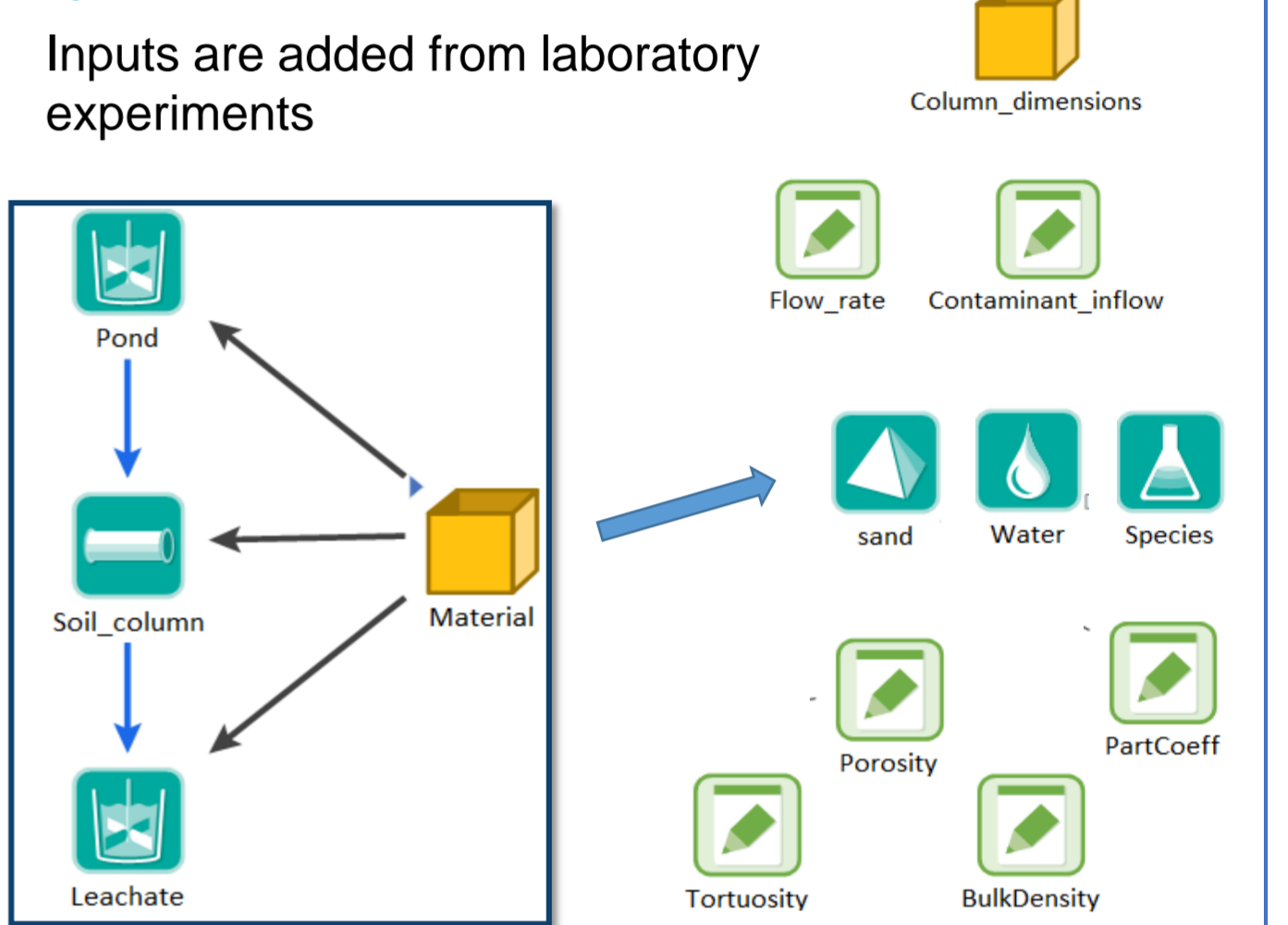
- Matrix → Quartz sand
- Contaminants → NTO and DNAN
- Analysis → HPLC-DAD

Methodology:

a) Laboratory experiment

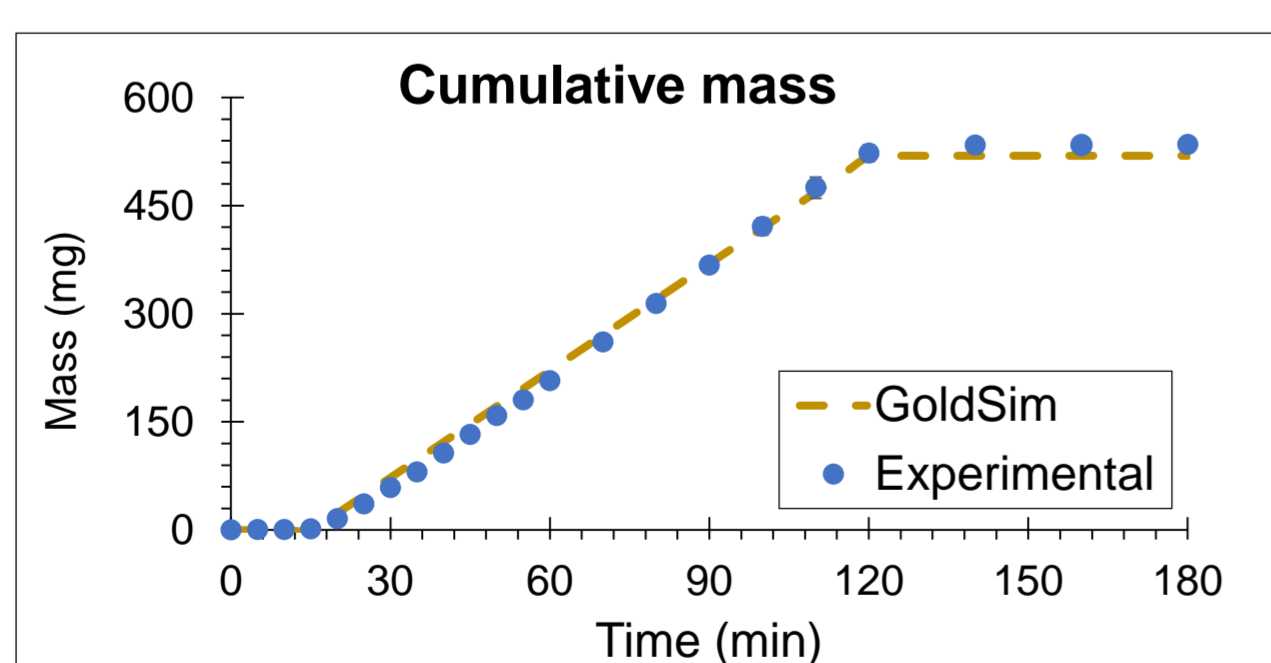
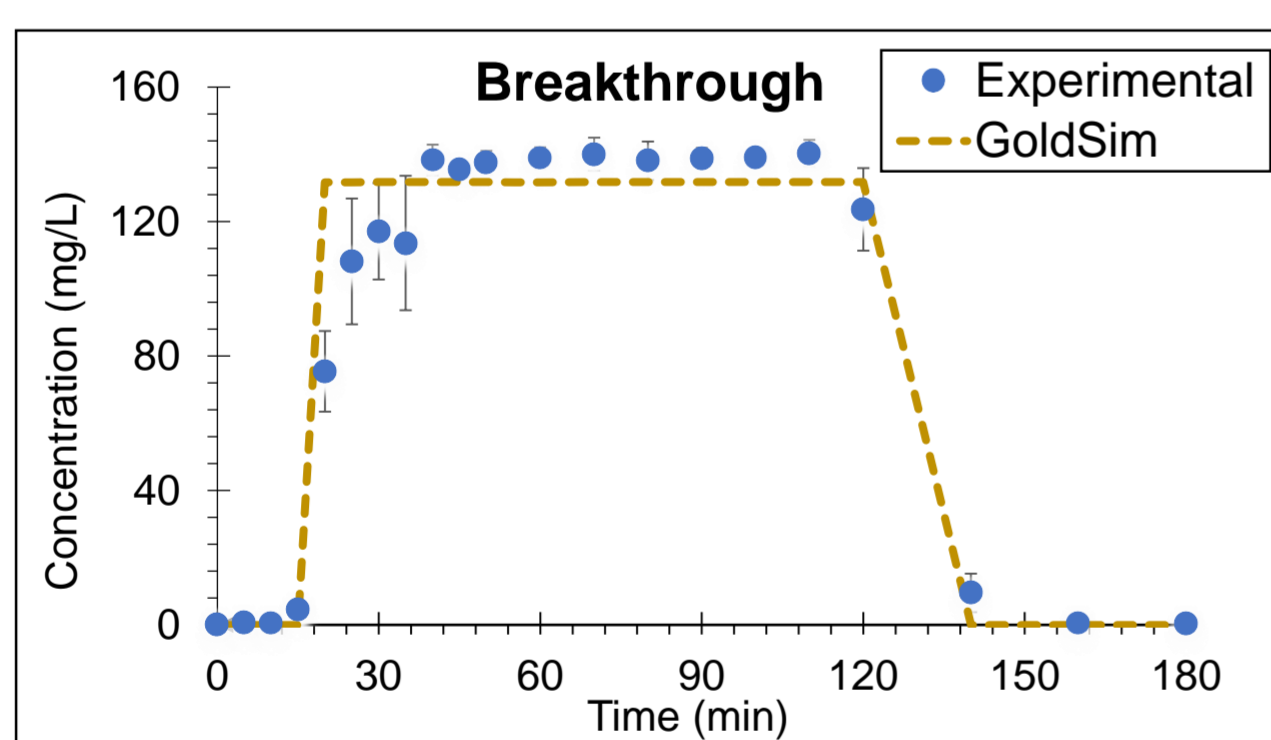


b) GoldSim simulation

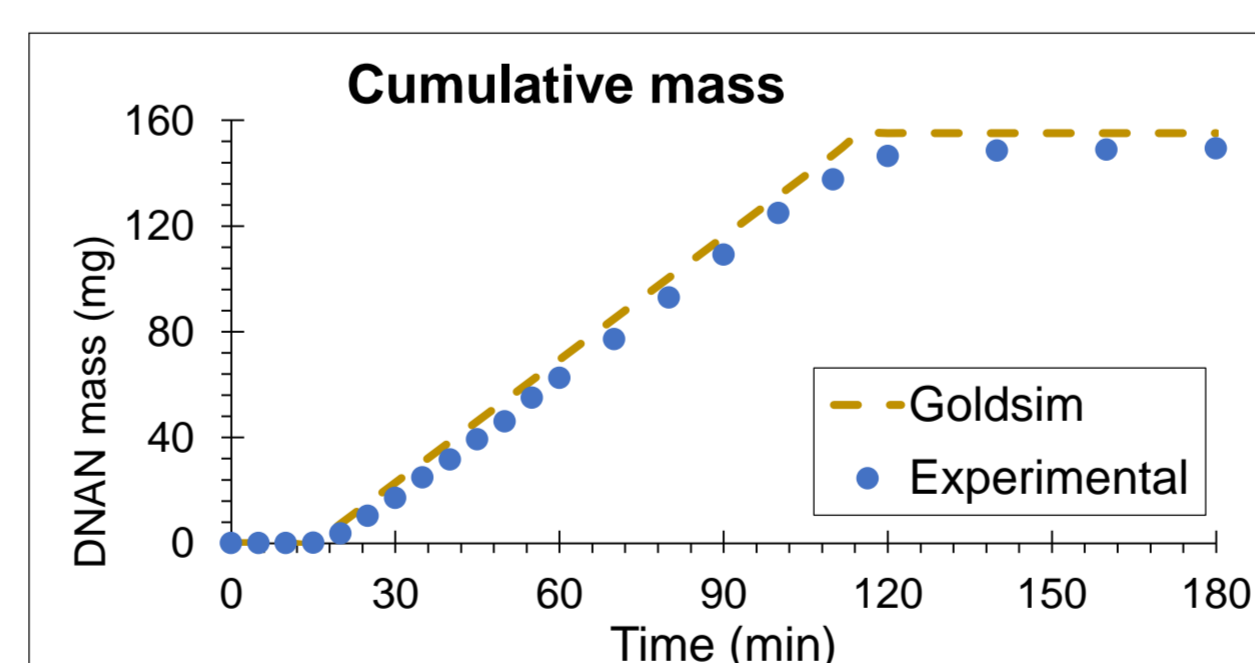
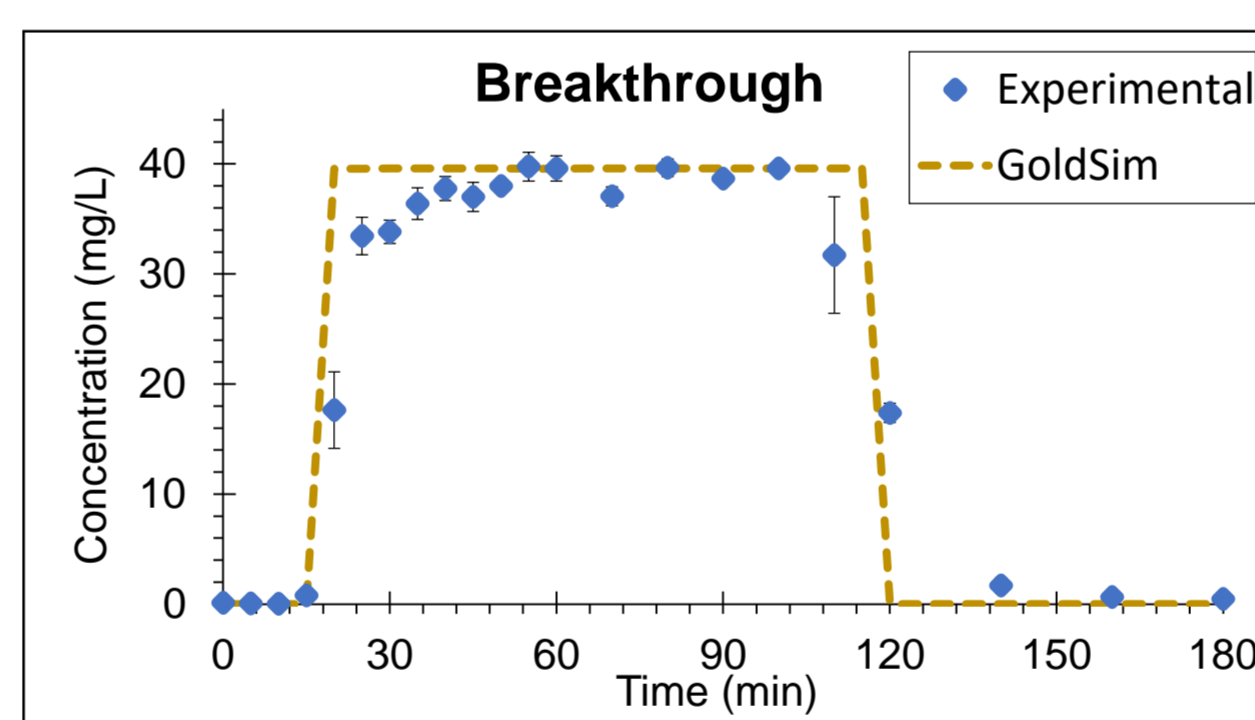


Results

NTO

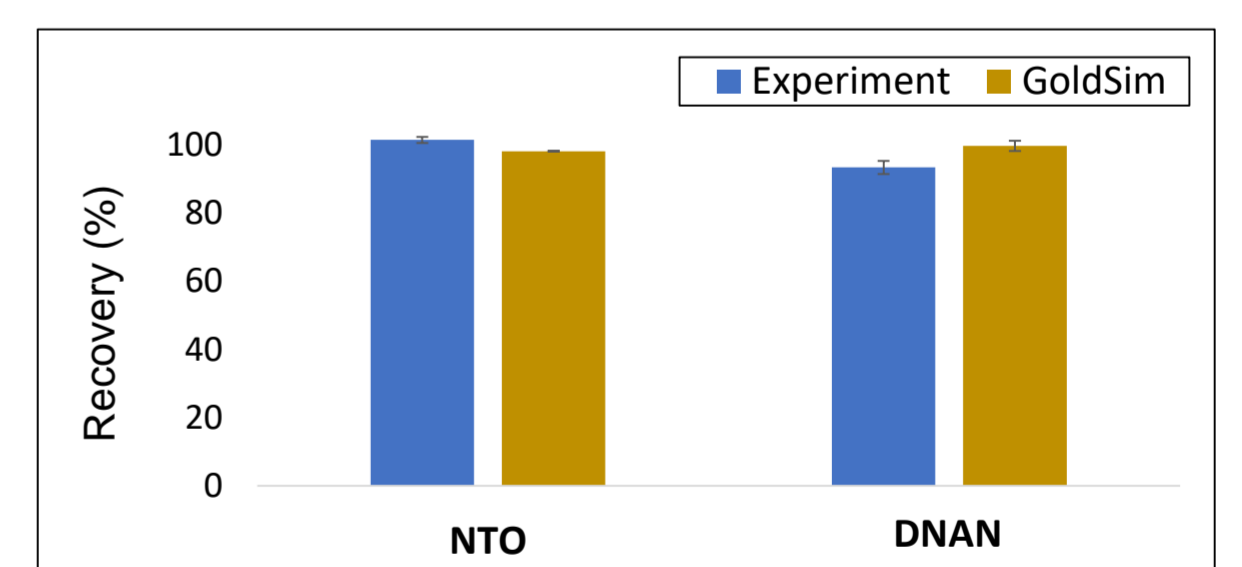


DNAN



Mass recovery

Approach	NTO (%)	DNAN (%)
Experimental	101.37 ± 0.90	93.3 ± 1.9
GoldSim	98.05 ± 0.13	99.6 ± 1.5



- Almost all NTO and DNAN was recovered
- Results are very similar between simulation and experiments
- Experiments show a larger standard deviation due to mass loss and systematic error during the performance

Conclusions

- The models created in GoldSim to predict NTO and DNAN breakthrough in quartz sand successfully simulated the column experiments. Therefore, quartz sand will be used as a control when testing different soil types.
- Parameters need to be experimentally tested in advance for creating new and better representative models of real environments.
- GoldSim simulations need further development to determine whether GoldSim is able to simulate mixtures of explosive compounds in more complex soils.