# Adsorption of Munitions Constituents via Cellulose, Cellulose Triacetate, Chitin, and Chitosan




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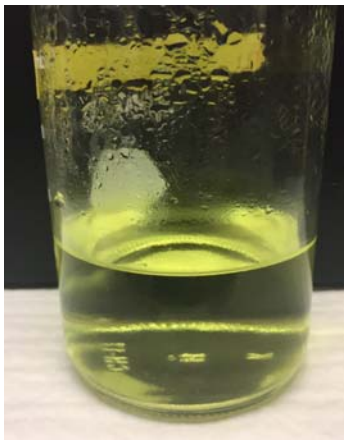
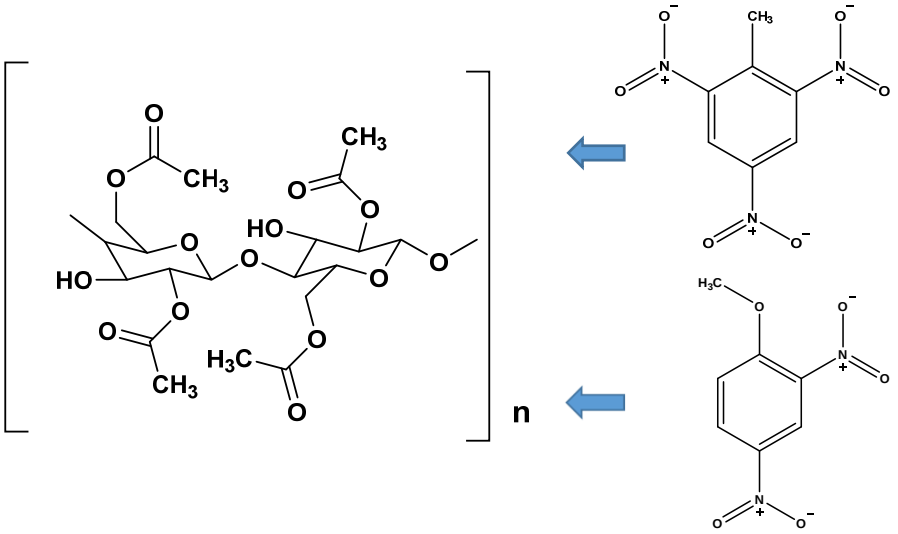
# Executive Summary

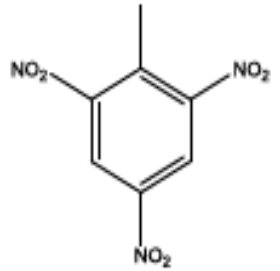
- Background
  - Insensitive munitions
    - Benefits
    - Environmental Concerns
  - Treatment Technologies
- Evaluations and Discussion
  - Adsorptive Removal
  - Isotherm Models
- Conclusions



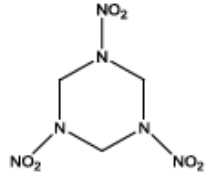


# Munitions Constituents

**Traditional Munitions**

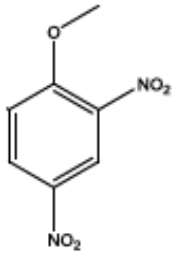


2,4,6-trinitrotoluene (TNT)

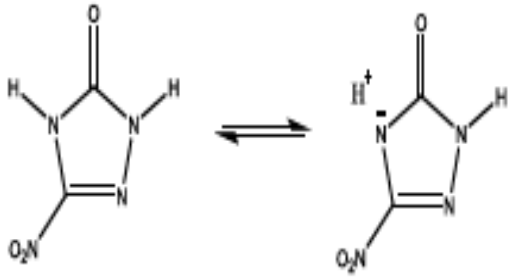


Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)

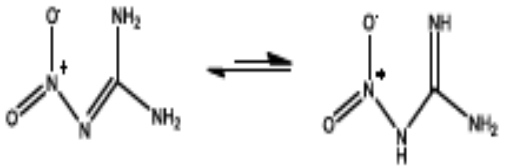
**Insensitive Munitions**



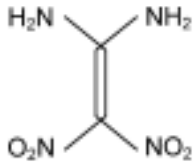
2,4-dinitroanisole (DNAN)



Nitrotriazolone (NTO)



Nitroguanidine (NQ)

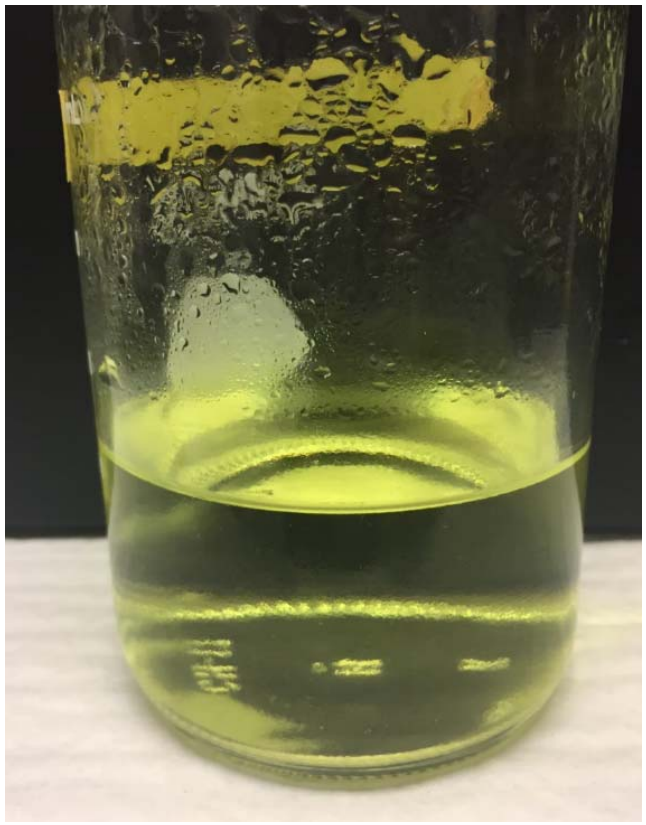


1,1-diamino-2,2-dinitroethene (FOX-7)

- Insensitive munitions (IMs) are currently being evaluated as alternatives to traditional munitions
- IM formulations contain more than one constituent

# IM Properties

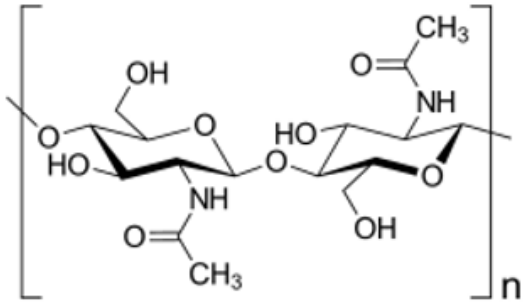
| Compound | Aqueous Solubility (mg/L) |
|---|---|
| NTO | 12,800 (19 $^{o}$C) |
| NQ | 4,100 (26 $^{o}$C) |
| DNAN | 280 (25 $^{o}$C) |
| TNT | 130 (20 $^{o}$C) |
| RDX | 43.2 (25 $^{o}$C) |



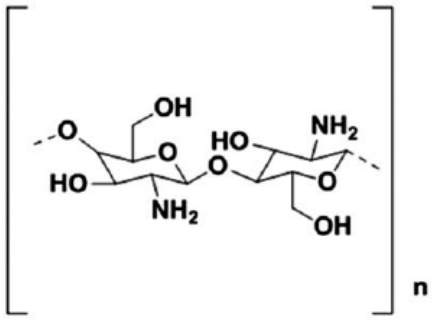
- Yellow color associated with IM formulations
- pKa of NTO = 3.76

# Polysaccharide Adsorbents

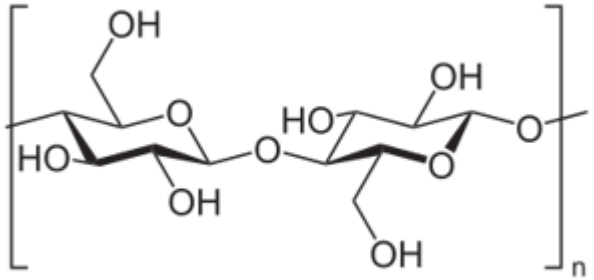
- Cellulose and chitin are two most abundant biopolymers in the world
- Derivatives formed from acetylation and deacetylation processes



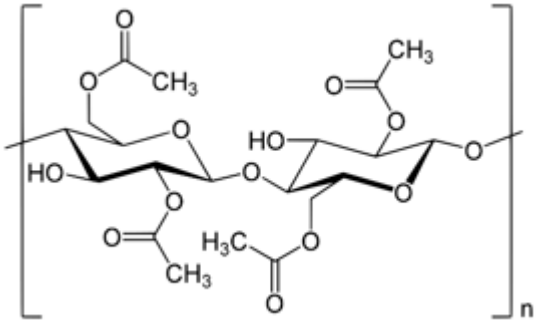
Chitin



Chitosan



Cellulose

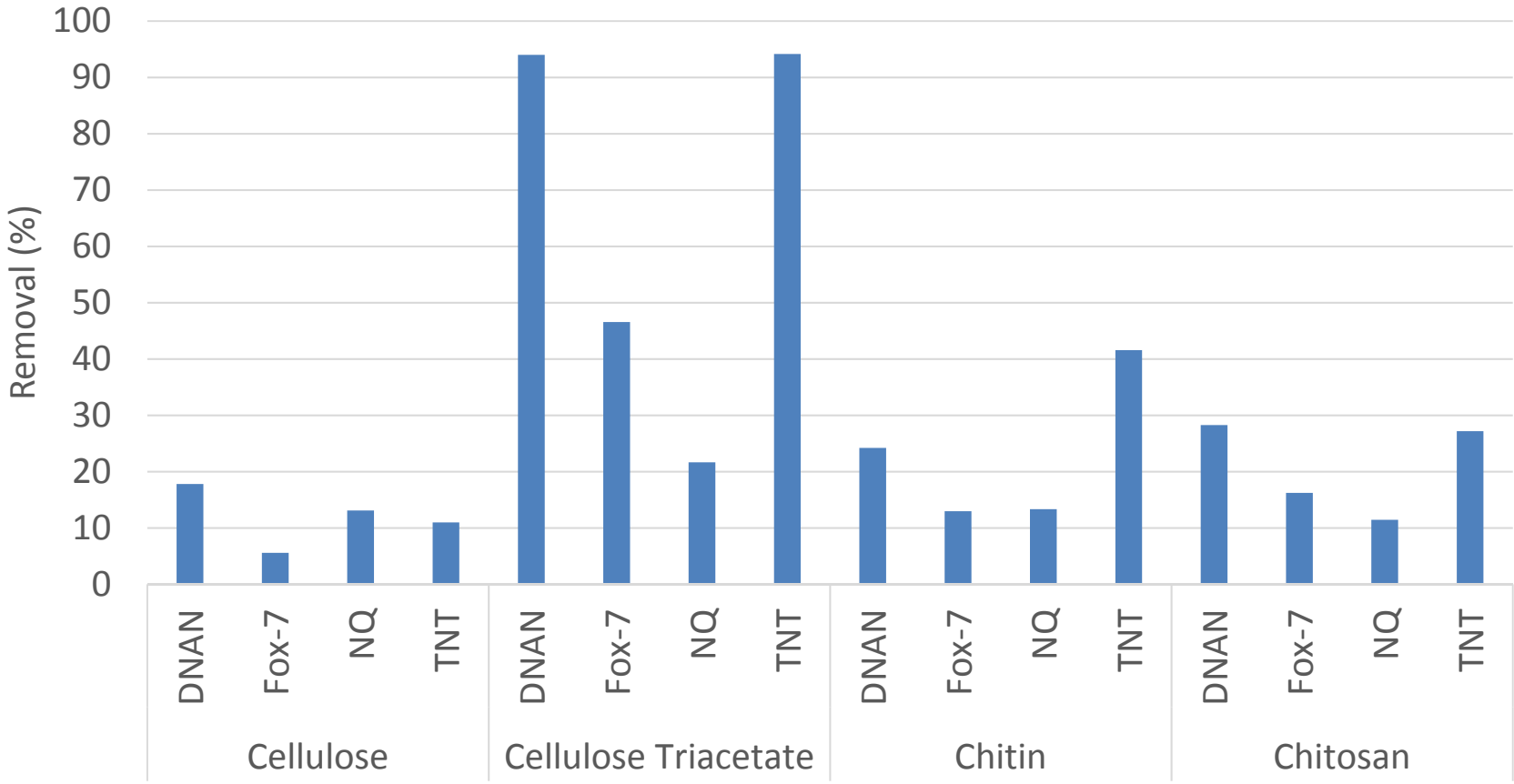


Cellulose Acetate

# Scope

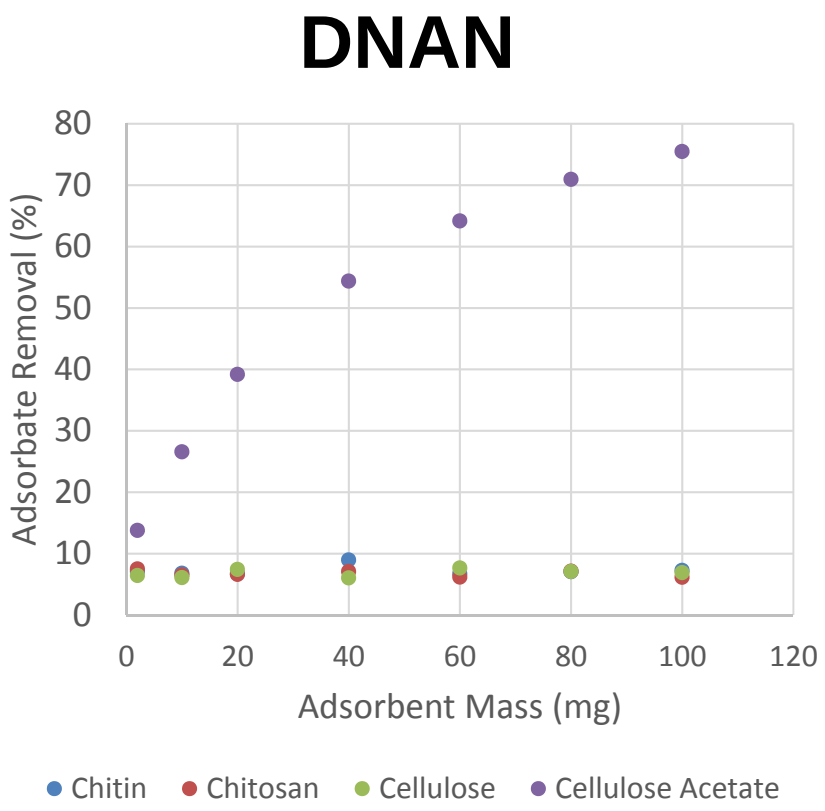
- Proof-of-concept evaluation
  - 10 mL aliquots of 2-mg/L solution vs. 500 mg of each adsorbent
    - DNAN
    - NQ
    - TNT
    - FOX-7
- Preparation and evaluation of isotherms
  - Successful adsorbate-adsorbent mixtures

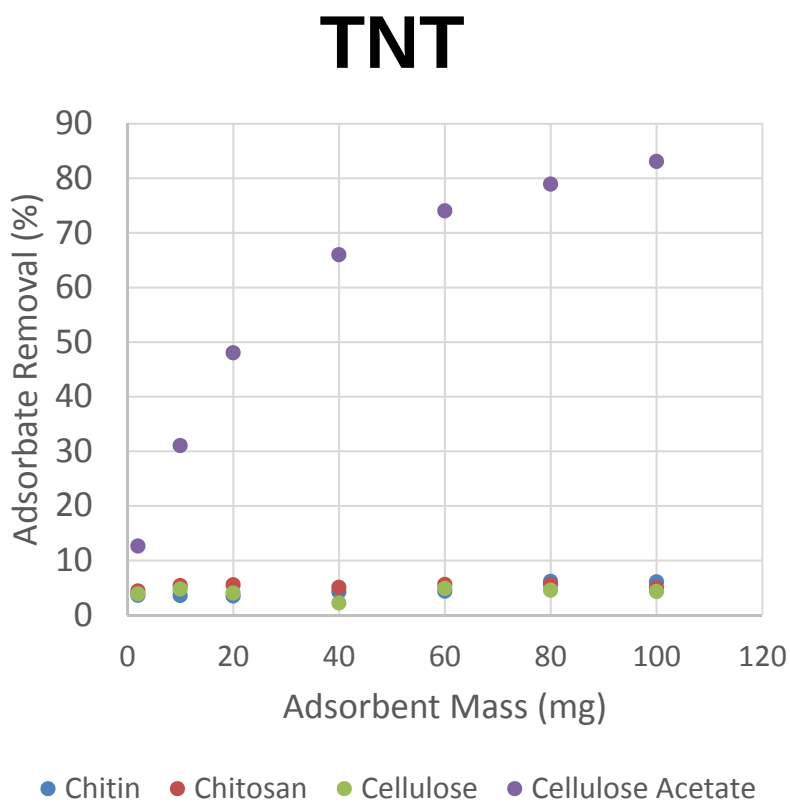
# Proof-of-concept Evaluation




- Definitive adsorption of DNAN and TNT via cellulose triacetate.
- Chitin and chitosan show potential adsorption of TNT.

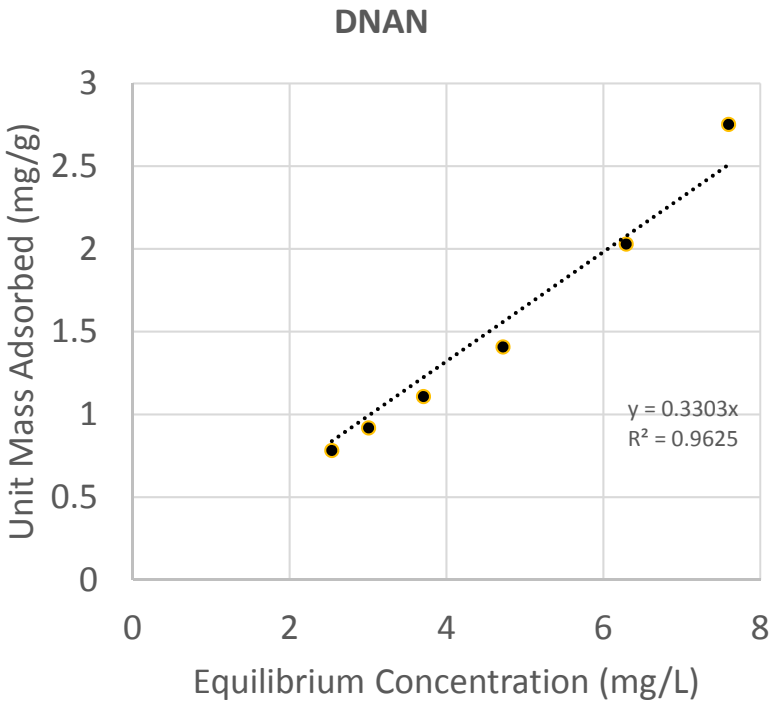
# Preparation of Isotherms

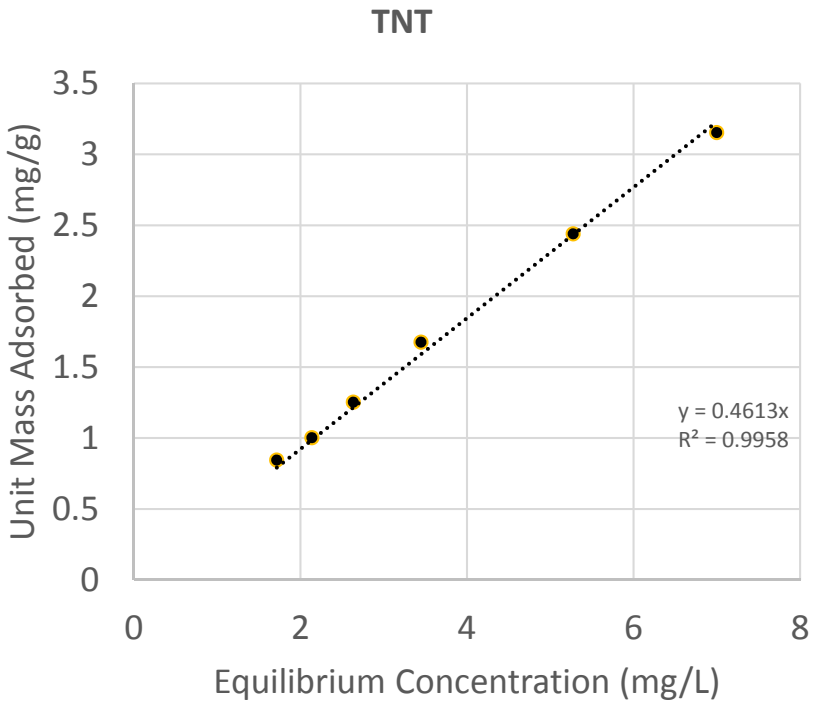



- 10-mL aliquots of 10-mg/L solutions vs. various adsorbent masses
- Only cellulose acetate showed observable adsorption trend

# Cellulose Triacetate Isotherms




| Compound | Distribution Coefficient (mL/g) |
|---|---|
| DNAN | 330.3 |
| TNT | 461.3 |

# Discussion and Next Steps

- DNAN and TNT display high affinity for cellulose triacetate.
  - Linear adsorption models applicable
  - Moderate removal of FOX-7 via cellulose triacetate
  - Electron-withdrawing groups cause adsorption
- All adsorbents show very low affinity for NQ and inconsistency for NTO
  - NTO is currently undergoing evaluation
- Next steps
  - Evaluate polysaccharides with electron-withdrawing groups to optimize removal
  - Produce adsorbents for removal of each IM

# Applications

- Utilization within industrial base for process water treatment
- In-situ surface water treatment technology for training ranges
- Sustainable alternatives to GAC and destructive processes

# Conclusions

- Cellulose, chitin, and chitosan are ineffective at removing IMs from solution
- Cellulose triacetate is an effective adsorbent for DNAN and TNT
- NTO speciation provides inconsistent adsorption results
- No material evaluated in this study successfully removed NQ from solution
- Associated Journal Article:
  - Gurtowski, L.A., C.S. Griggs, V.G. Gude, M.K. Shukla. 2017. An integrated theoretical and experimental investigation of insensitive munition compounds adsorption on cellulose, cellulose triacetate, chitin and chitosan surfaces. *J. of Environmental Sciences*.

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