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# KNOO

## Modelling the rheology of magnox sludges

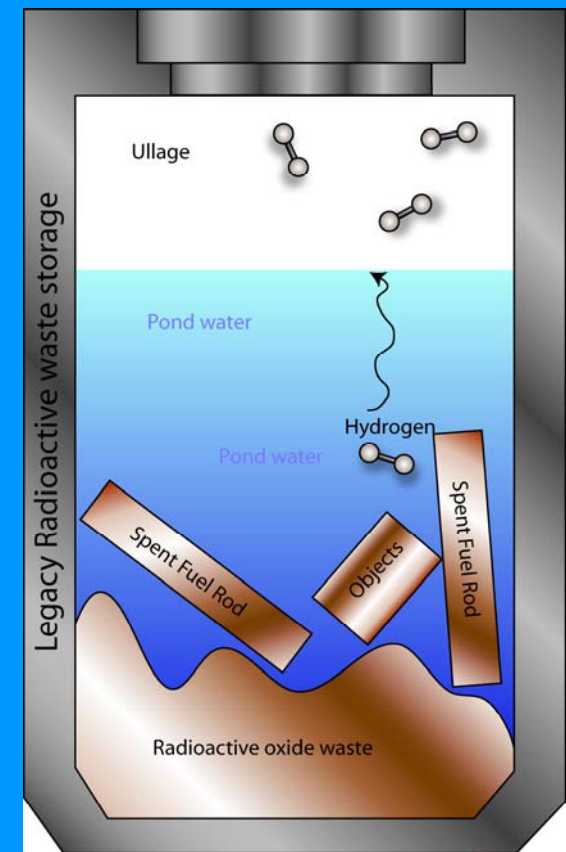
Karl Travis + PDRA



# Mesoscale modelling of Magnox sludges

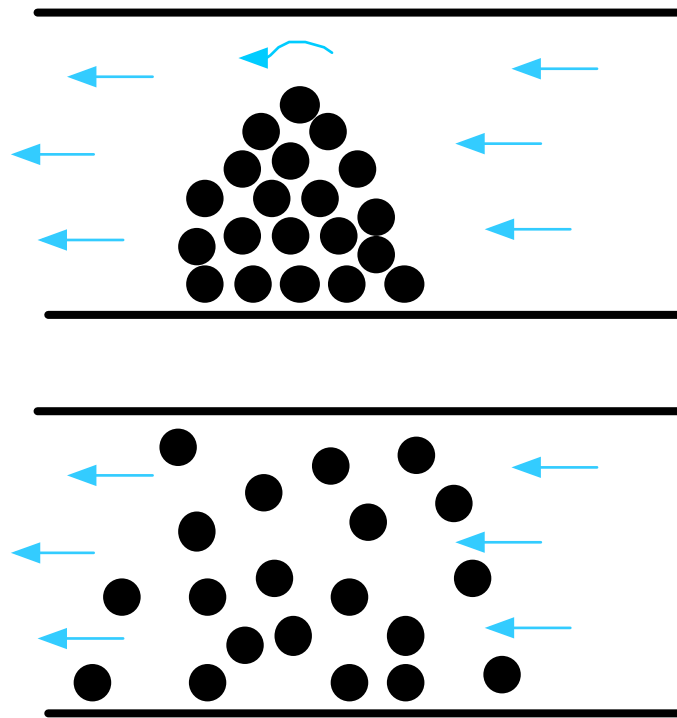
## Legacy waste issues

- Legacy wastes at Sellafield Site
  - Sludges in storage tanks and ponds
- Recovery/ storage operations
  - Pumping/ Squeezing
  - Grouting in waste package



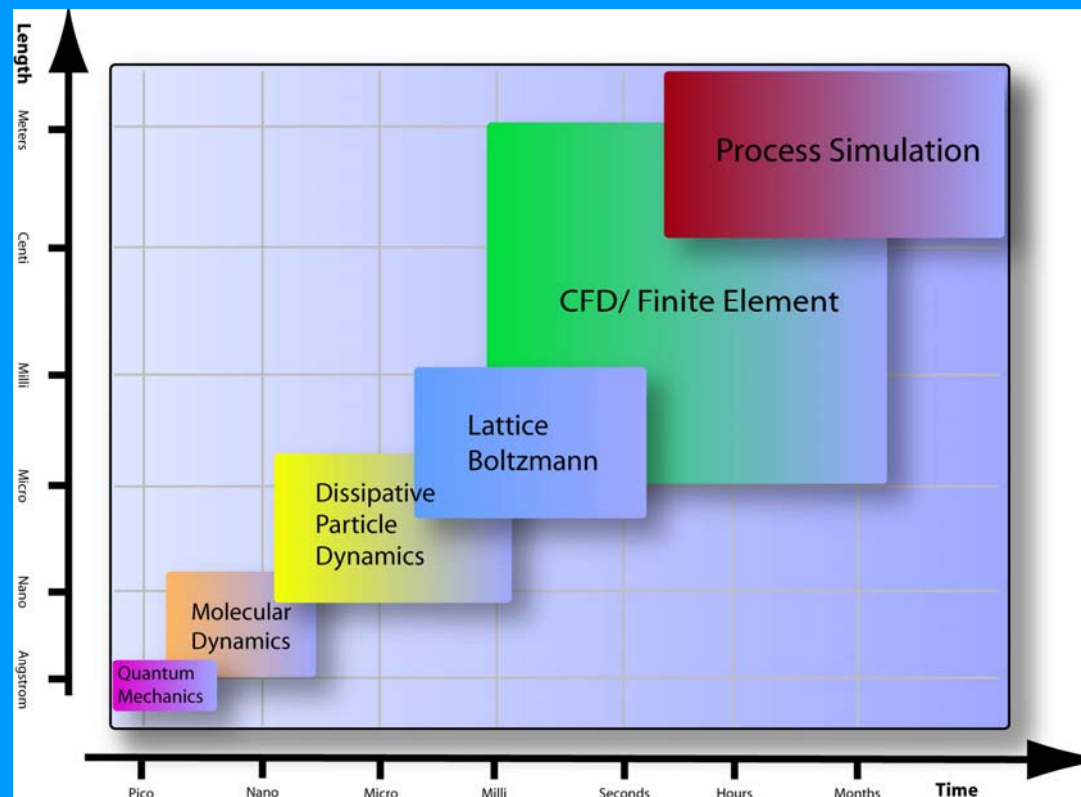


- Use dissipative particle dynamics (DPD) to simulate the mechanical break-up and mobilisation of  $\text{Mg}(\text{OH})_2$  sludge particles.





- Dissipative Particle Dynamics is one component of a hierarchy of modelling methods.
- Good for multiphase systems.
- Chemistry can be built into the model.





# The DPD method

- Forces pairwise additive

$$F_i = \sum_{i \neq j} (F_{ij}^C + F_{ij}^D + F_{ij}^R)$$

- Conservative

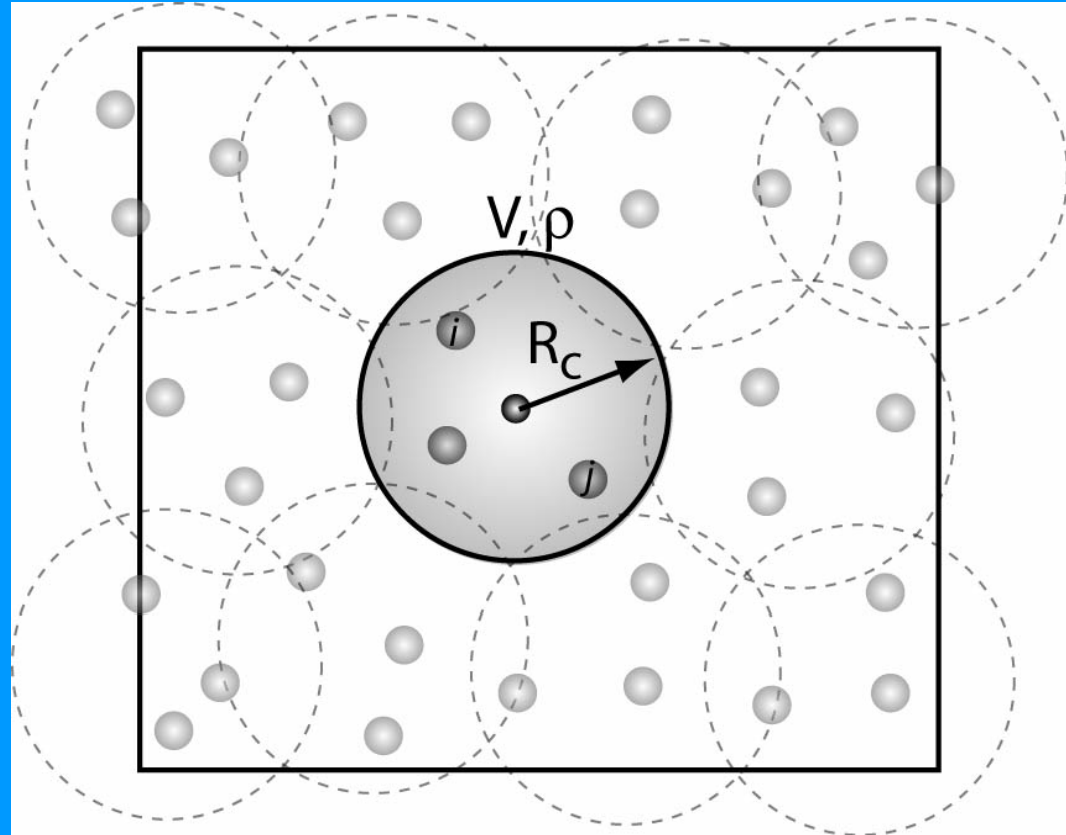
$$F_{ij}^C = a\omega^C(r_{ij})\hat{r}_{ij}$$

- Dissipative

$$F_{ij}^D = -\zeta\omega^D(r_{ij})(v_{ij} \cdot \hat{r}_{ij})\hat{r}_{ij}$$

- Random

$$F_{ij}^R = \sigma\omega^R(r_{ij})\xi_{ij}\hat{r}_{ij}$$





## Work plan

- Build different boundary conditions into DPD code
- Obtain DPD conservative interaction parameters for sludge particles using combination of experimental and molecular mechanics data.
- Explore how size and shape of particles affects their dispersal under various flow conditions.

PDRA - Dr Martin Whittle: start date 02/01/07, duration 18 months.



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# KNOO Cements for encapsulation of flocs and zeolitic adsorbents

NB Milestone and Y Bai



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## AIM

- Development of a cementing system compatible with floccs such as magnesium hydroxide/carbonate and zeolitic based ion exchangers

## STAFF

- 1 2-year PDRA Dr Y Bai appointed May 2006



# Current encapsulation cements

- ILW and LLW are currently encapsulated with composite OPC cements containing large amounts of supplementary cementing materials such as blast furnace slag (BFS) or pulverised fuel ash (PFA)
- These have been chosen primarily to reduce heat output during hydration of the cement which can reach temperatures in excess of 100°C in the centre of the drum



## Advantages of OPC based composites

- Rapid strength development – hardens within 24 hours
- High pH (<12) renders many heavy metal hydroxides insoluble
- Properties reasonably well known
- Compatible with many wastes
- Matrix has relatively low permeability



## Disadvantages of OPC composites

- High pH causes problems with reactive metals such as Al, Mg, U
- These corrode in alkaline matrix giving expansive corrosion products and liberate large amounts of hydrogen
- Alkaline pore solution attacks and destroys zeolites releasing adsorbed ions
- Reaction can be reduced by addition of PFA but not BFS
- Reaction probably caused by large amounts of free water held in capillary pores as only limited hydration occurs in OPC composites



## Disadvantages of OPC composites II

- When these composites are used with iron floc, very high w/s ratios are required to allow mixing ( typically 0.85 instead of 0.37)
- Results in porous, (53%) weak matrix which could be subject to leaching
- Pores filled with water and can lead to waste/matix interactions such as corrosion



## Alternative cement requirements

- Moderate pH to avoid reactions with waste
- Hydration reaction to remove excess pore water
- Low heat of hydration/reaction when hardening
- Relatively impervious matrix
- Compatibility with waste



# Possible alternatives I

- Calcium sulhoaluminate cement
  - pH ~ 10.5 -11
  - Binds large quantities of water in hydration product ettringite
  - Ettringite also can be substituted with many anions and cations in structure making it a good host
  - Preliminary experiments show ideal for Al
  - Further work needed to determine durability
  - Disadvantage - cement must be imported from China



# Possible alternatives II

- Sulphate activated Slag
  - pH remains low at ~10.5
  - Hydration product is a mixture of ettringite and C-S-H
  - Preliminary experiments give good results for setting
  - Can be made from UK slag. Similar to supersulphated cement made to British Standard and also available in Europe
  - Collaboration with China brings a Chinese worker here from November to take the work further
  - Preliminary results presented at conference in Switzerland in July



# Future work

- Further characterisation of activated slag system
- Introduction of simulated wastes - sludges and zeolites
- Durability and leaching studies



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# NCH - KNOO

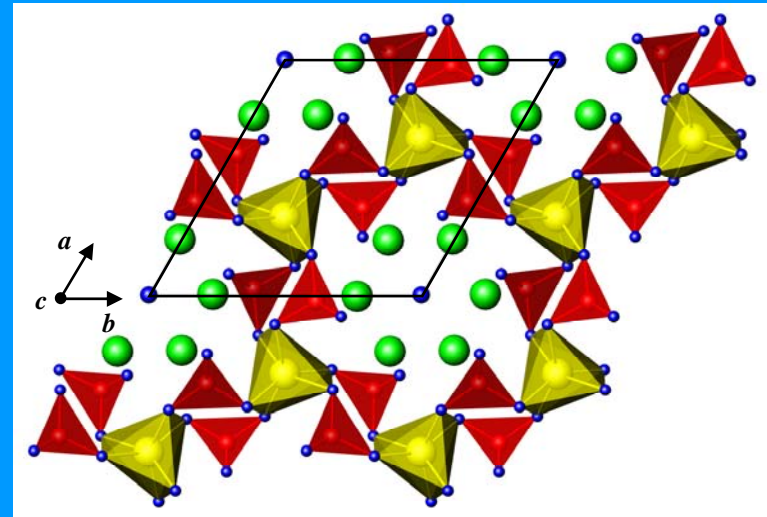
Neil Hyatt

Department of Engineering Materials, The University of Sheffield



# Ceramic and glass-ceramic wasteforms

- **Initial focus on apatite systems:**
  - high chemical flexibility
  - halide immobilisation
- $A_{4-x}Ln_{6+x}(SiO_4)_{6-y}(PO_4)_y(X,O)_2$
- A = Li, Na, Mg, Ca, Sr, Ba, Pb or Cd,  
X = Cl or I and Ln = trivalent lanthanide



- **Single phase ceramics:** halide in solid solution
- **Glass-ceramics:** partition halide into ceramic, fission products into glass
- **Hot Isostatic Pressing:** to counter halide volatility
- **PDRA appointment:** interviews completed 13/09, appointment offered



# Ceramic and glass-ceramic wasteforms

- **First phase of work:**
- Order and install Hot Isostatic Press
- Determine suitable target compositions
- Determine composition / structure / microstructure / durability relations
  
- **Hot Isostatic Press: AIP6-30H**
  - Small scale unit
  - Similar system to that used by ANSTO & Nexia
- **Specifications:** up to 2000°C and 200 MPa

