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4TU.

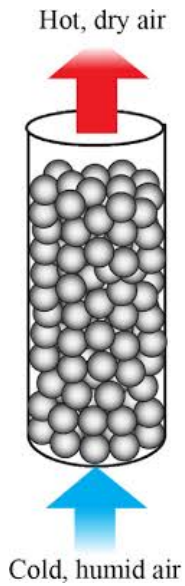
Thermo-Chemically Active Granular Materials



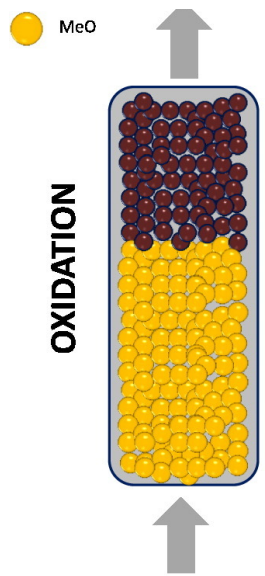

Thomas Weinhart, Mina Shahi,
Ruud van Ommen, Anthony Thornton

Background & Motivation

- Granular materials play a crucial role in many industries (chemical, energy, pharma, etc.)
- This often involves **chemo-thermo-mechanical** processes. (heat exchange, hydration, chemical reactions, catalysts).



Heat storage



Solid-gas reactions

- No open-source software exists to simulate such processes.
- Our project aims to bridge this gap.

Aim & Project overview

Aim of ChemGrain

- Develop an open-source simulation tool for particle simulations with chemo-thermal properties.
- Validate and apply the model to industrially relevant cases.
- Write follow-up grant.

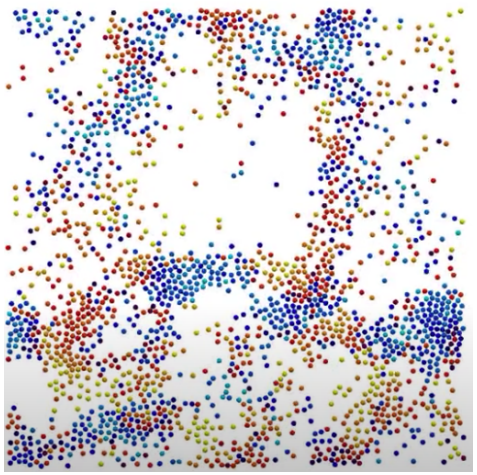
Project overview

- **Thomas Weinhart, Anthony Thornton**: Model development in MercuryDPM
- **Ruud van Ommen**: Experimental validation with ozone decomposition
- **Mina Shahi**: Experimental validation with salt hydration, Application to thermochemical heat storage

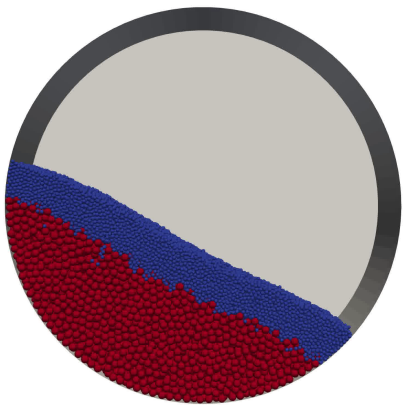
Particle simulations

- Simulates motion of many particles by applying forces.
- Implemented open-source in MERCURYDPM
- Coupled to gas-phase via drag relations.

Free-cooling gas



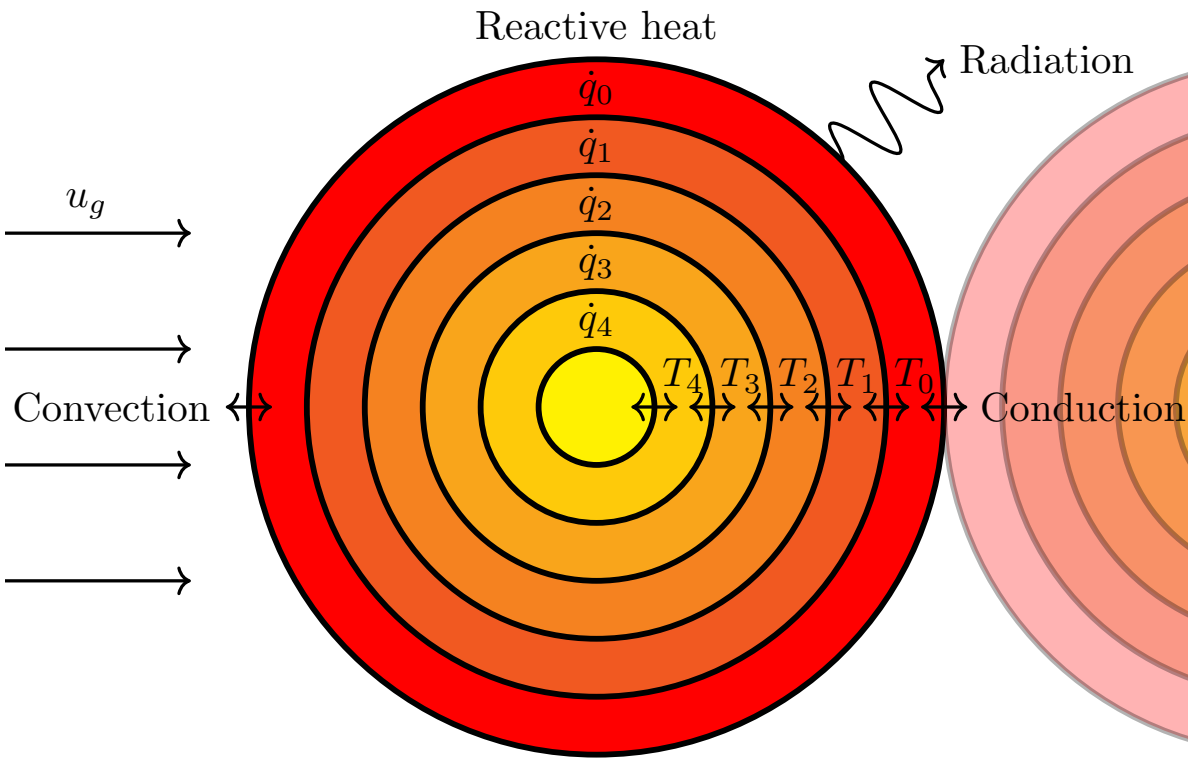
Rotating drum



Silo flow

Modelling Heat Transfer

- Start with shell model.
- Solve the heat transfer equation $\frac{\partial \rho c_p T}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \lambda_{\text{eff}} \frac{\partial T}{\partial r}\right) + \dot{q}_{react}$ with boundary conditions $-\lambda_{\text{eff}} \frac{\partial T}{\partial r}\Big|_{r=R} = \dot{q}_{\text{conv}} + \dot{q}_{\text{rad}} + \dot{q}_{\text{cond}}$.

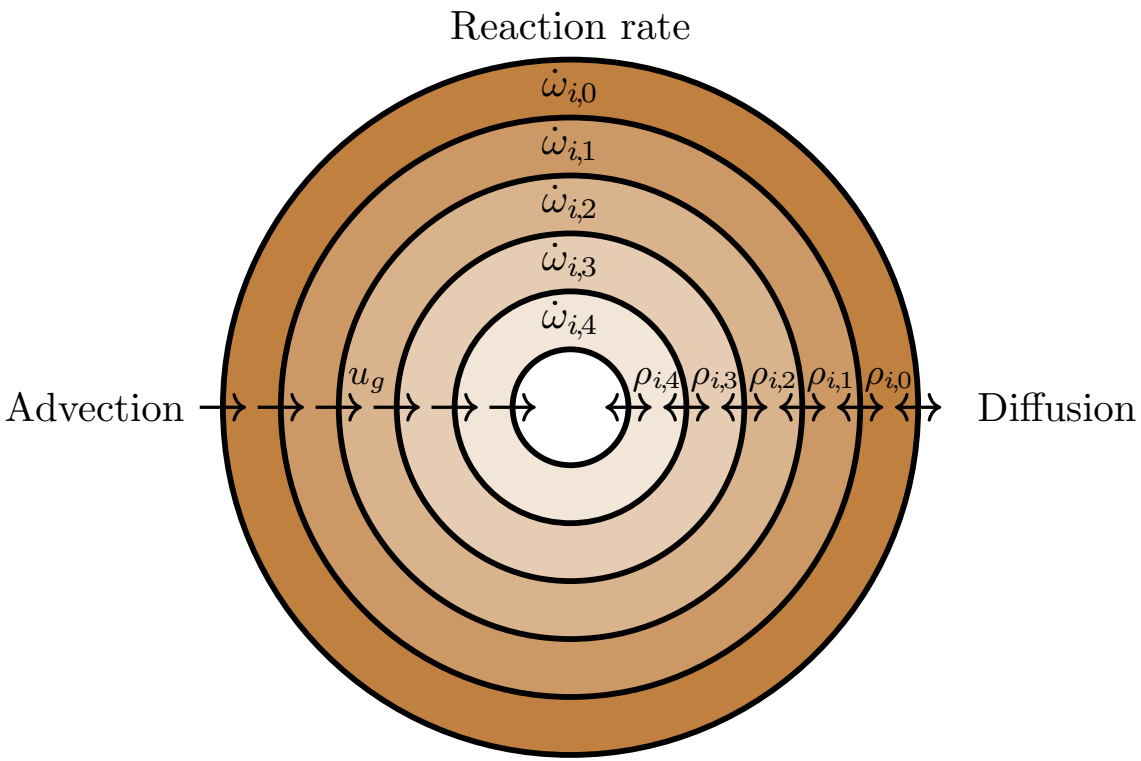


Modelling Mass Transfer

- Solve the species density equation

$$\frac{\partial(\epsilon\rho_i)}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\rho_i u_g\right) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D_i \epsilon \frac{\partial}{\partial r}\rho_i\right) + \epsilon\dot{\omega}_i$$

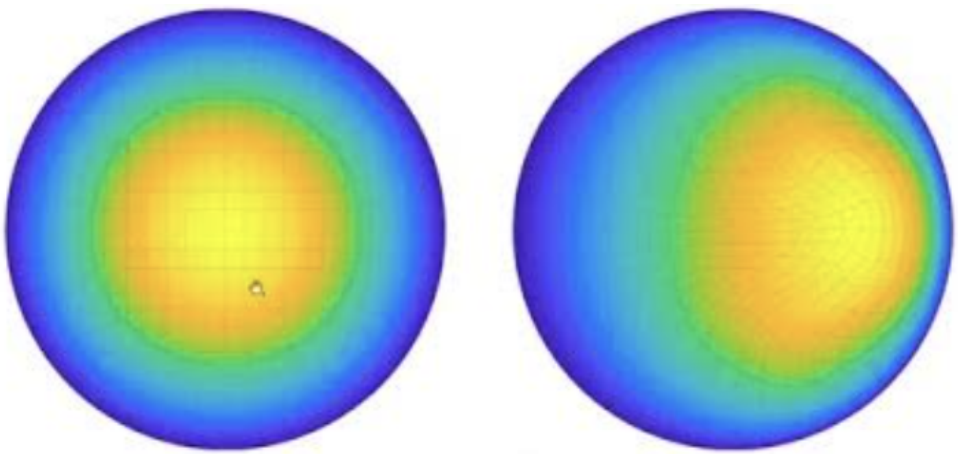
with boundary conditions $-D_i \frac{\partial \rho_i}{\partial r}\Big|_{r=R} = A_s\left(\dot{m}_{\text{diff}} + \dot{m}_{\text{adv}}\right).$



Modelling shape

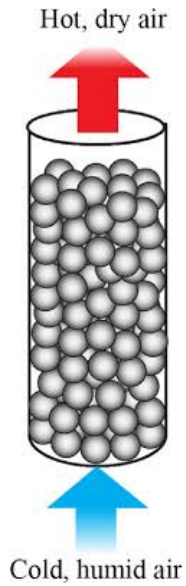
- Extend shell model to non-spherical shapes using level-sets.

- Future: Generalise using model order reduction (decompose into dominant modes).



Validation: salt hydration

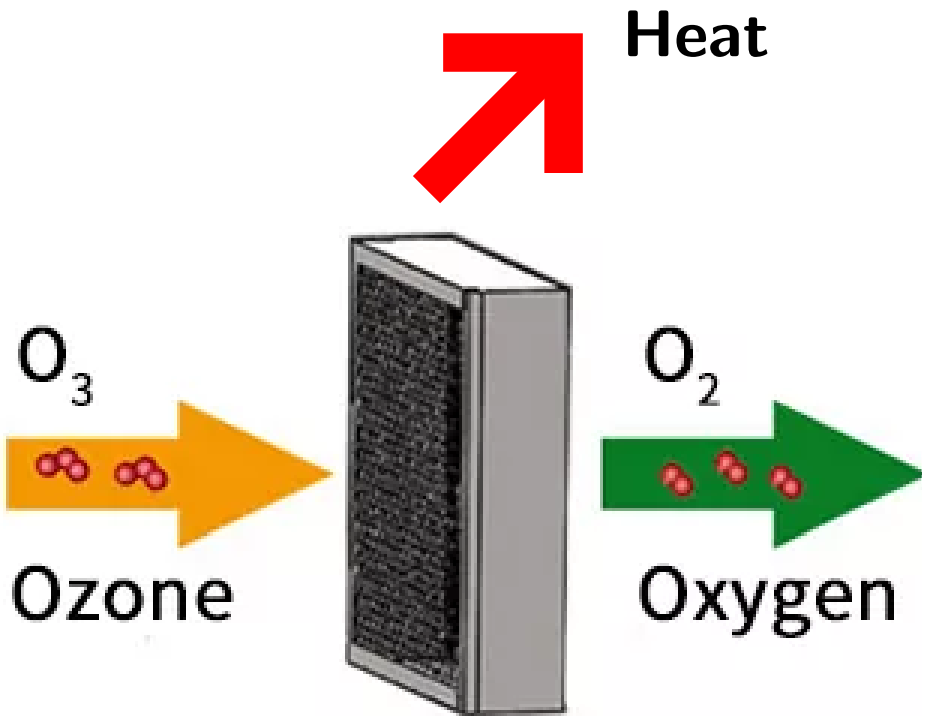
- Validation using salt (de-)hydration in a heat exchanger.
- Involves solid-gas reactions with phase change.
- Demonstration for real-world application.



Heat exchange, Hydration

Validation: ozone decomposition

- Experimental validation: ozone decomposition in a packed-bed reactor.
- Demonstrates chemical reactions and heat generation on catalyst surfaces.



Ozone decomposition

Outlook

- This project lays the foundation for further research into thermo-chemical granular systems.
- Apply for funding to extend model's capabilities/applications:
  - More complex chemical reactions.
  - Experimental validation at larger scales.
  - Use of sustainable materials.
  - Real-world applications in energy storage, catalysis, process optimisation.

Let's drive innovation in sustainable energy systems!

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