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Potential Applications for Inverse Methods in CFD and Heat Transfer at NNL

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The Role of Inverse Problems and Optimisation in Uncertainty Quantification
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DEPARTMENT OF ENERGY & CLIMATE CHANGE

Shareholder Executive
HM Government

From October 2013

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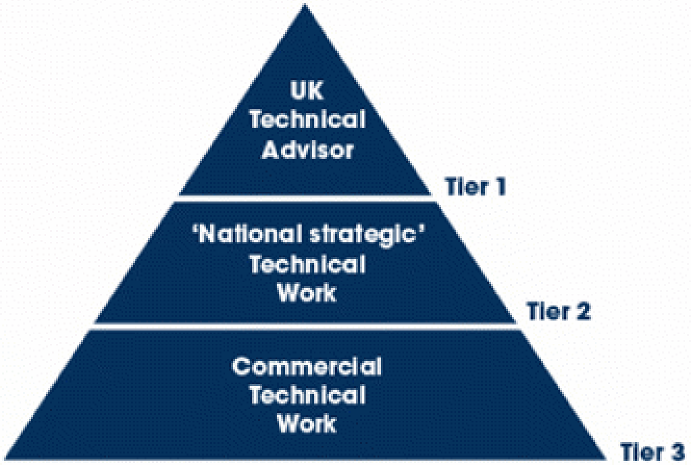
- National Laboratory Government for both UK and Industry
- Support to National R&D Programmes



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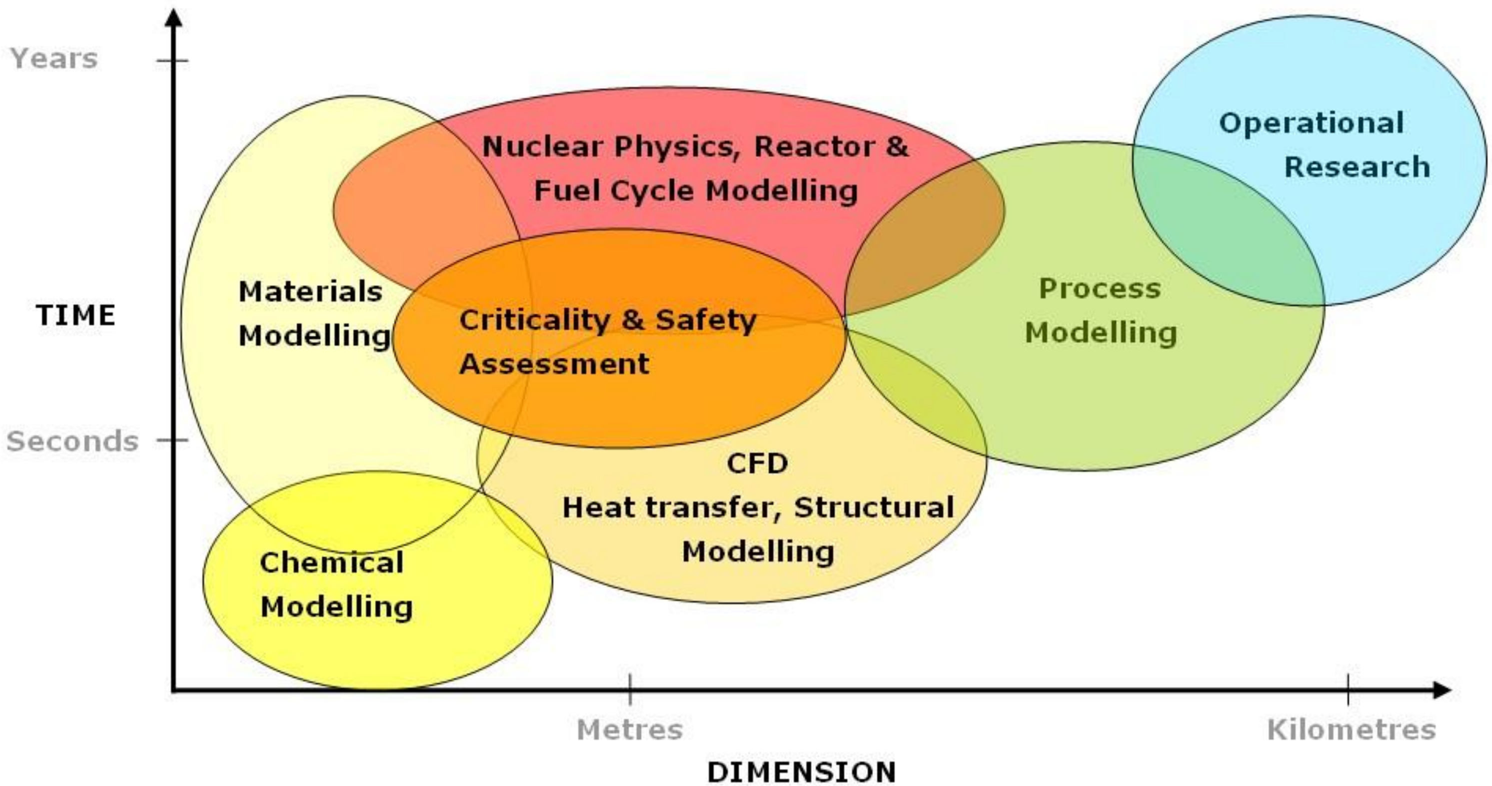
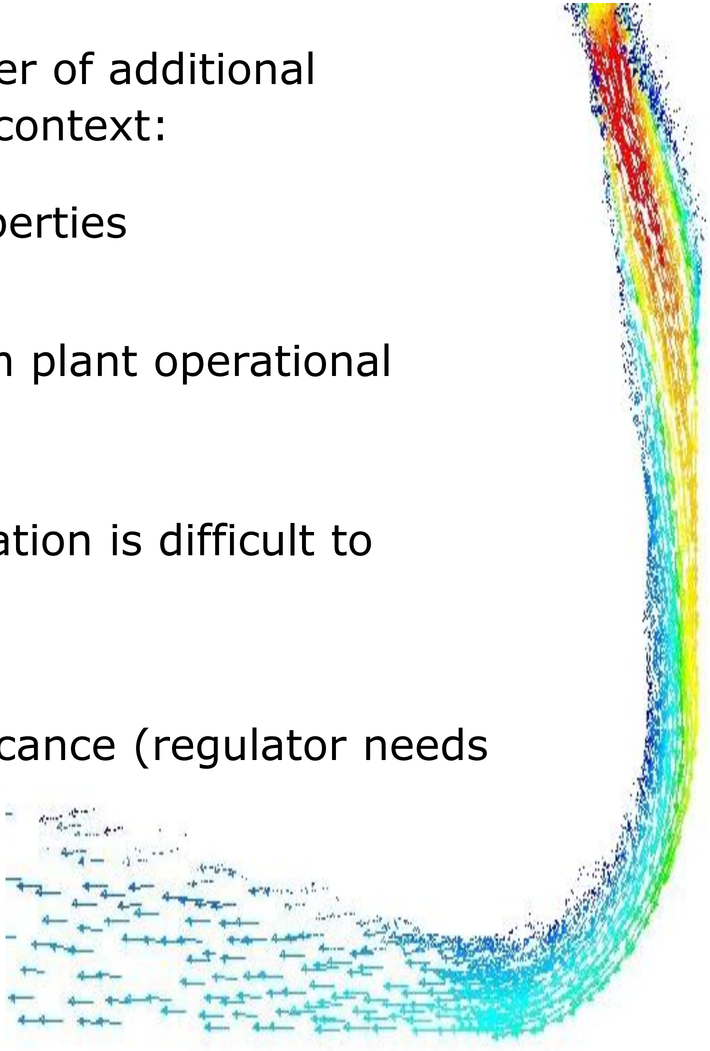
Modelling Capability at NNL



Challenges for Mathematical Modelling in the Nuclear Industry

Experience in NNL has shown that CFD has a number of additional challenges associated its application in the nuclear context:

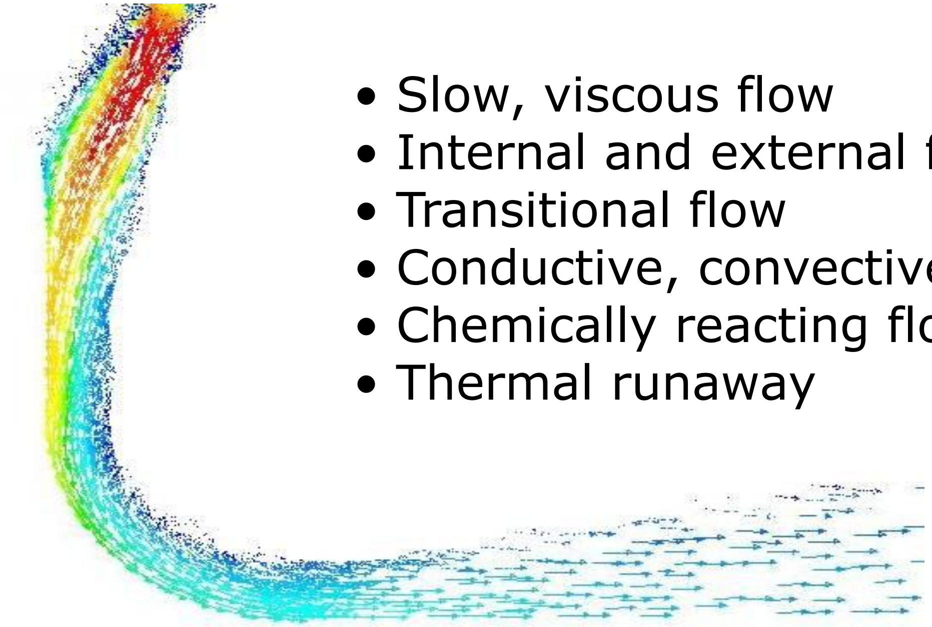
- Little information on material physical properties
- Difficult to define boundary conditions from plant operational parameters
- In many cases specific geometrical information is difficult to obtain
- Confidence in results is of particular significance (regulator needs to be convinced)
- Can Inverse Problem methodology help?



Range of Challenges (Fluid Flow and Heat Transfer)

At NNL, nearly all the fluid flow and heat transfer work delivered to date has been centred in the reprocessing and decommissioning areas.

The specific physics (and chemistry!) covers the following range:



- Slow, viscous flow
- Internal and external flow
- Transitional flow
- Conductive, convective and radiative heat transfer
- Chemically reacting flow
- Thermal runaway

Range of Challenges (Fluid Flow and Heat Transfer)

We can define a second order PDE to describe the evolution of many physical processes including heat transfer, fluid flow, mass transfer etc

From the Finite Volume perspective:

$$\frac{\partial}{\partial t}(\rho\phi) + \nabla.(\rho \mathbf{v}\phi) = \nabla.(\Gamma\nabla\phi) + S_{\phi}$$

unsteady convection diffusion source

Solution Methodologies

Three main categories exist depending on the complexity of the problem and the accuracy required

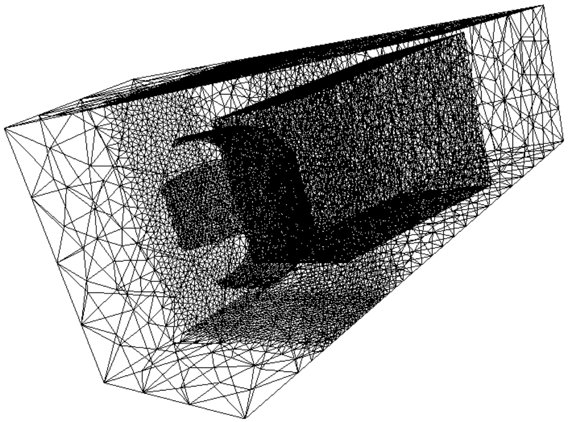
1. Hand calculations (e.g. heat conduction, force balance etc)
2. Lumped parameter (e.g. flow/heat transfer network analysis)
3. Large codes (e.g. Finite Volume – CFD, Finite element – stress analysis)

For (2) and (3) a discretisation step is required

$$\frac{\partial}{\partial t}(\rho\phi) + \nabla.(\rho \mathrm{v}\phi) = \nabla.(\Gamma\nabla\phi) + S_\phi$$

$$\downarrow$$

$$a_p\phi_p = \sum_{nb} a_i\phi_i + S_\phi$$



Inverse Methods

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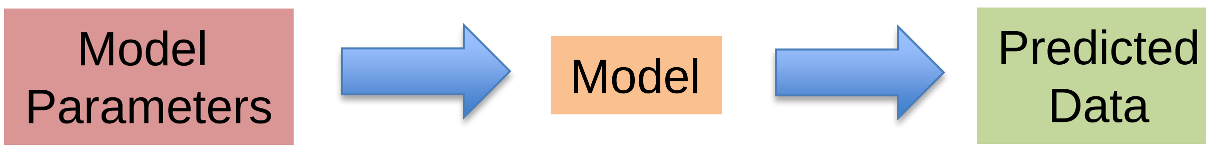
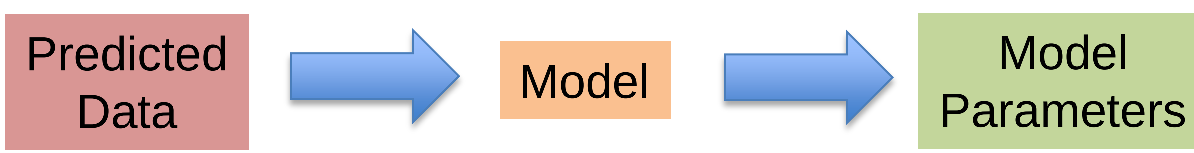
Forward Theory:



Inverse Theory:



Potential Applications
Boiling Heat Transfer (1)

- Establishing the operational lifetime of vessels in the nuclear industry is important for plant safety.

- Heat transfer plays an important part and calculations are undertaken to predict metal temperatures.

- Sometimes processes that govern thermal resistance in the liquid boundary layer are complex.

Potential Applications
Boiling Heat Transfer (2)

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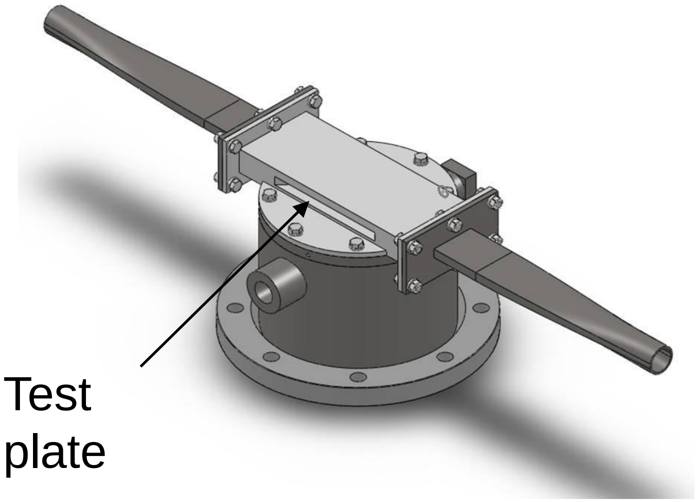
Work will be underway at the NNL Workington Laboratory to assess the change in heat transfer coefficient along a heated plate. The physics includes:

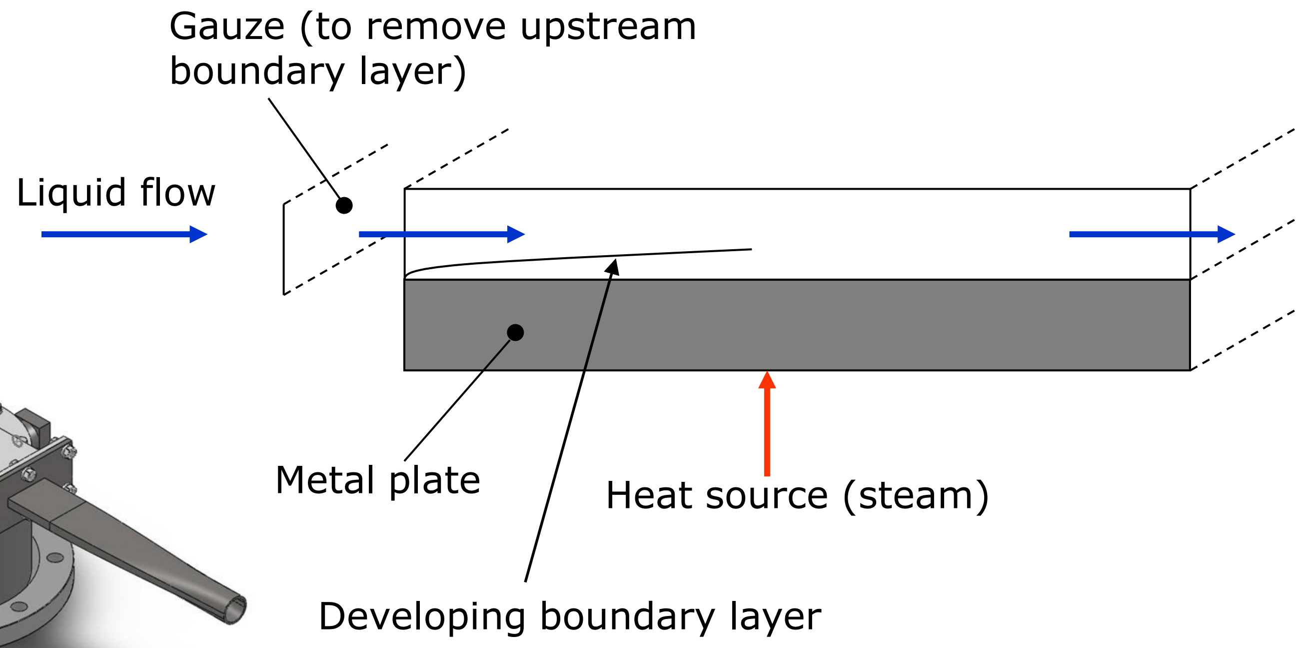
- Transition from laminar to turbulent flow
- Transition from convective to boiling heat transfer

The work will establish the correlation:

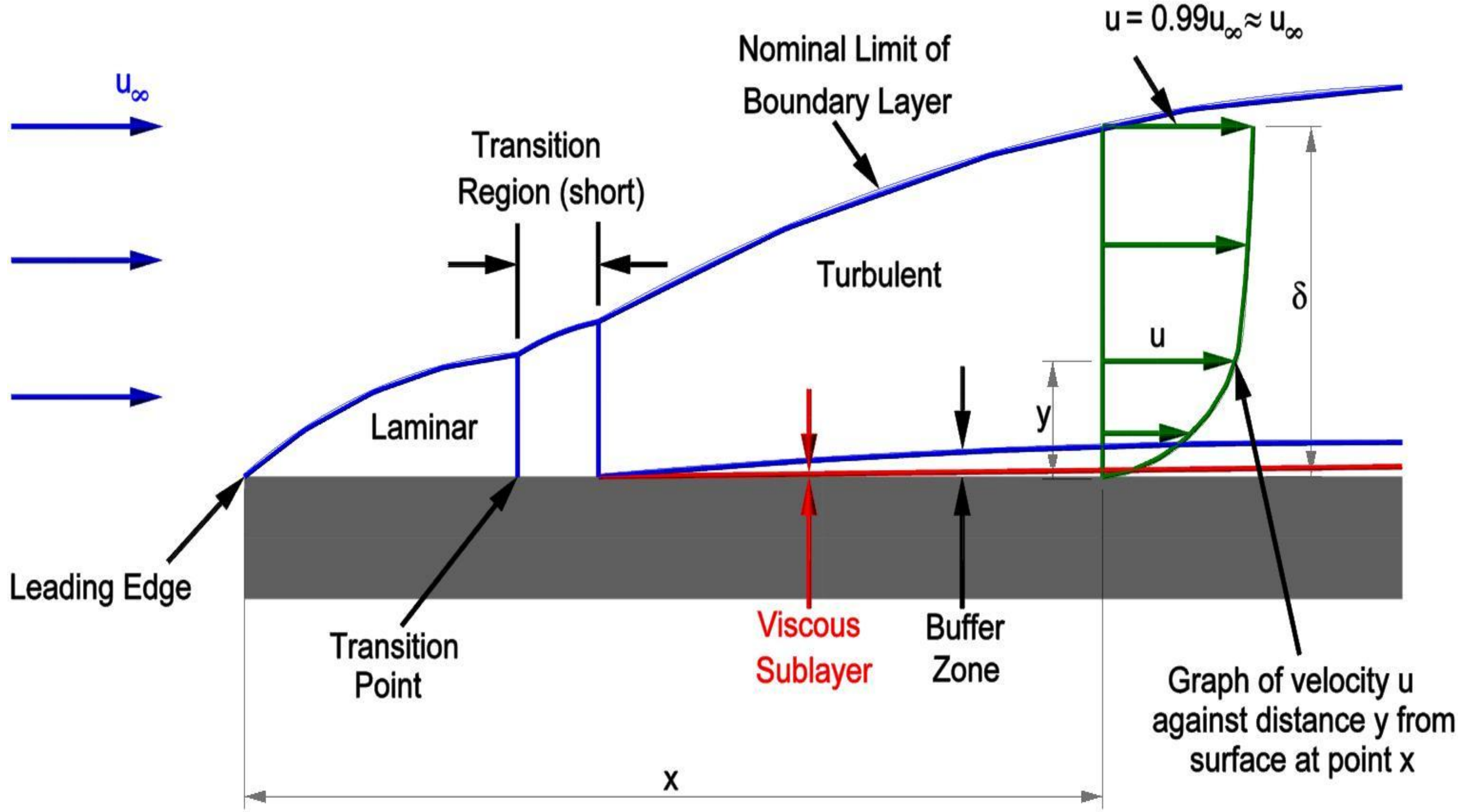
$$h = (C_1 h_{conv}^a + C_2 h_{boil}^b)^c$$

Potential Applications
Boiling Heat Transfer (3)





Potential Applications
Boiling Heat Transfer (4)



Potential Applications Boiling Heat Transfer (5)

- Thermocouples will be placed in the metal at various locations through the thickness of the plate and along the plate
- Can inverse methods be used to establish the variation in heat transfer coefficient along the plate?

Potential Applications
Corrosion and Hydrogen Generation (1)

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- Establishing the operational lifetime of vessels in the nuclear industry is important for plant safety.

- In some environments corrosion will take place with hydrogen gas evolved as a product of the chemical (Arrhenius) reaction.

- Hydrogen can also be produced as a result of radiolysis (molecular oxygen and hydrogen production as a result of fission)

Potential Applications
Corrosion and Hydrogen Generation (2)

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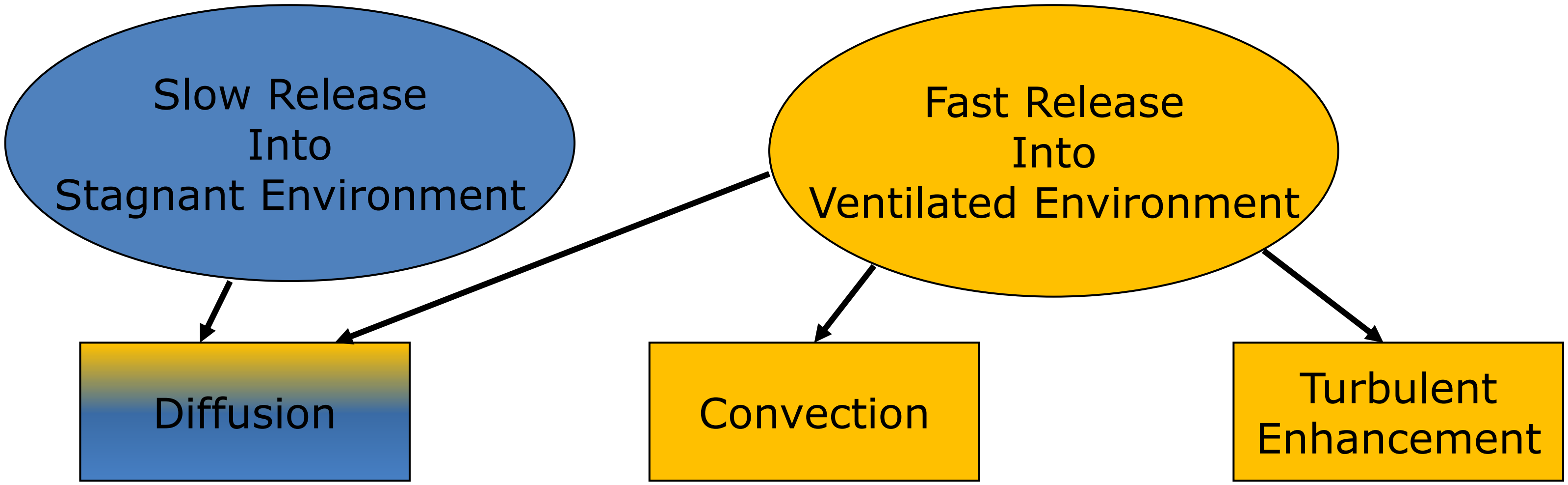
Underlying Physics:



Potential Applications
Corrosion and Hydrogen Generation (3)

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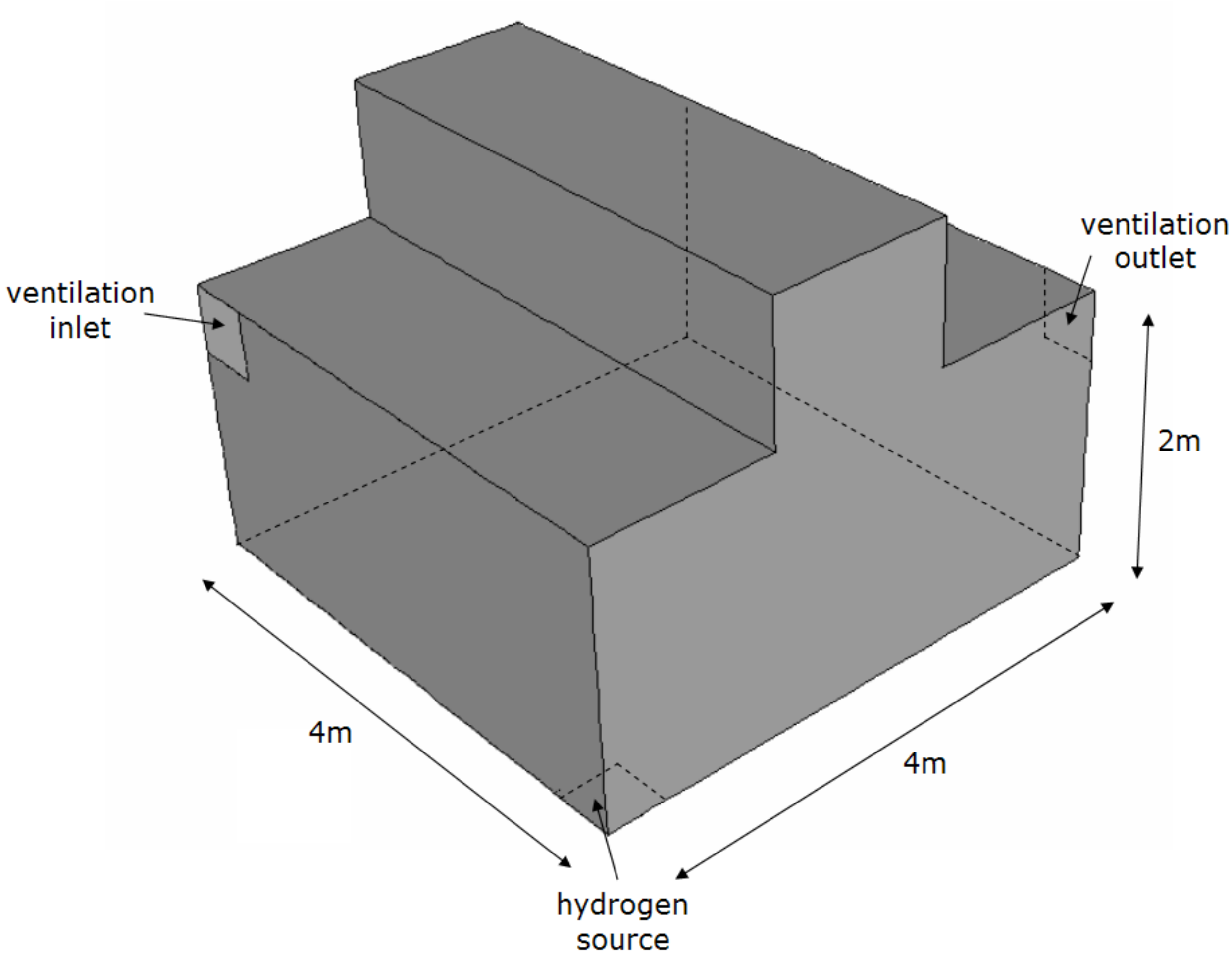
Test Case: Unsteady Release into a Ventilated Environment



Potential Applications
Corrosion and Hydrogen Generation (4)

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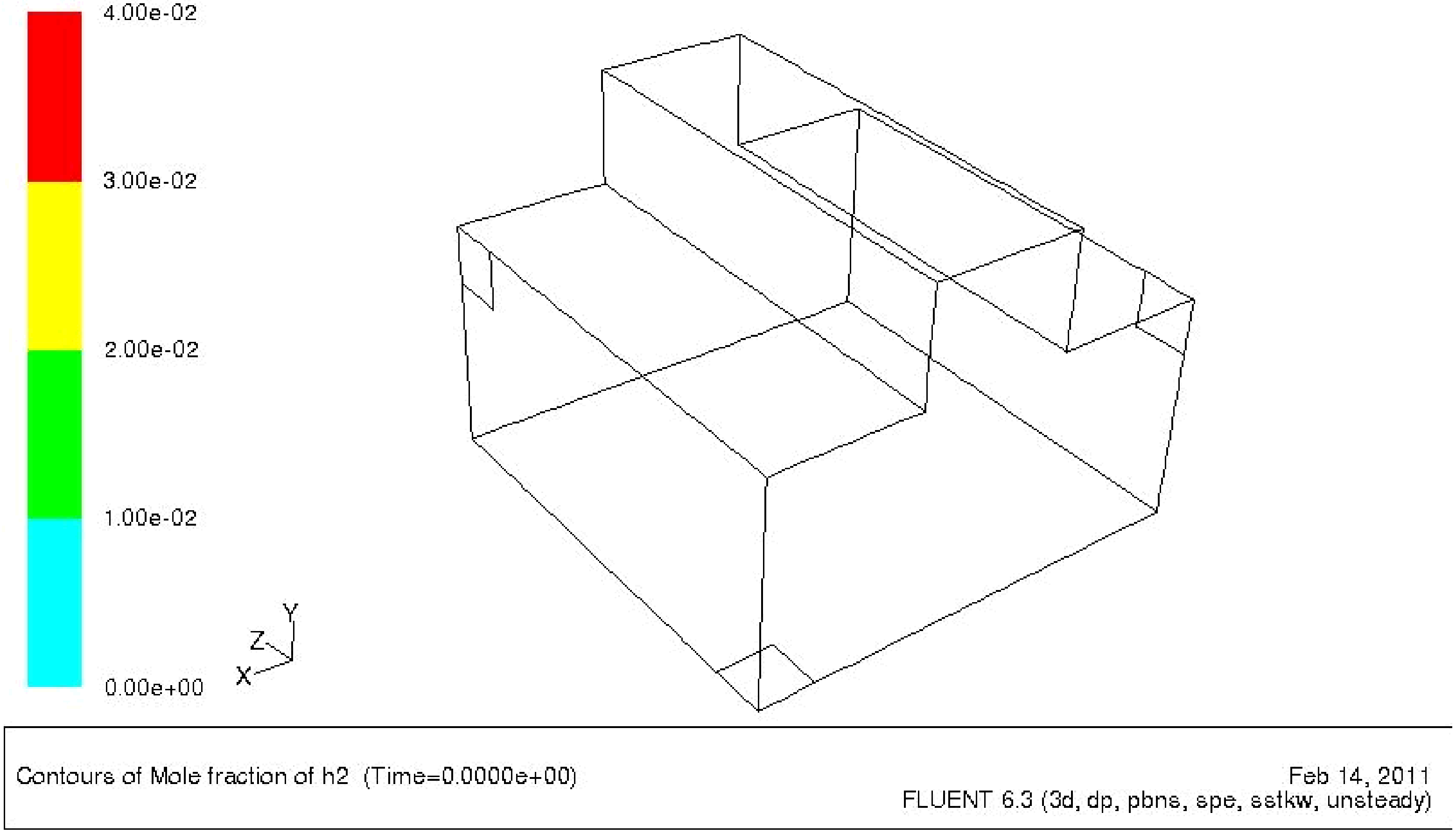
CFD Calculation: Mole Fraction Iso-surfaces



Potential Applications
Corrosion and Hydrogen Generation (5)

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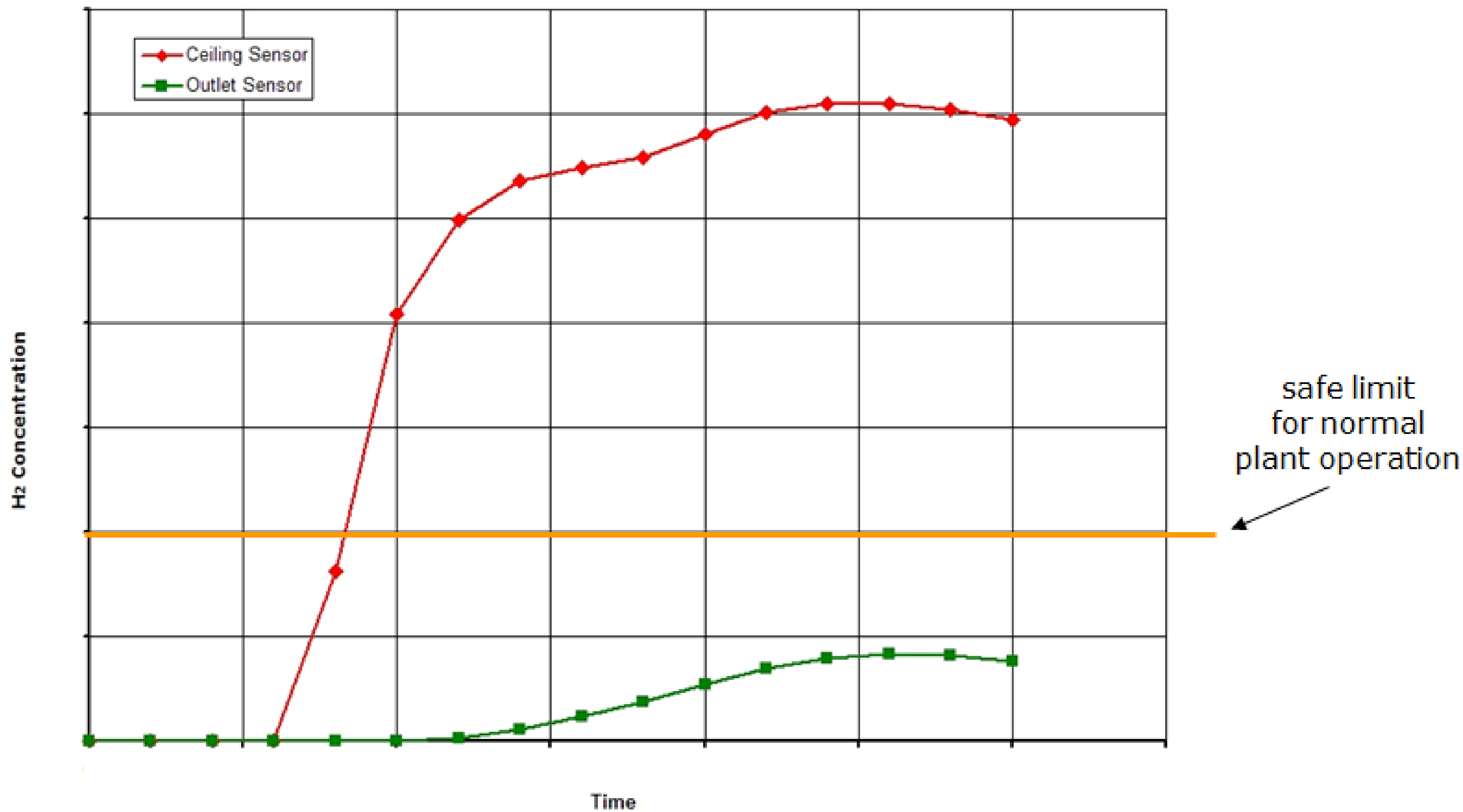
Predicted Sensor Concentrations



Potential Applications
Corrosion and Hydrogen Generation (6)

- CFD model/plant hydrogen monitoring can be used to give guidance on the amount of hydrogen released
- Can inverse methods be used to estimate the rate of corrosion experienced by the system?

Potential Applications
Glass Melter Analysis (2)

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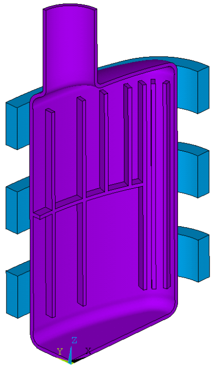
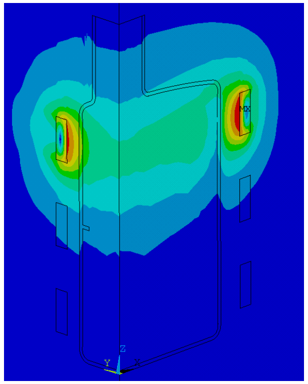
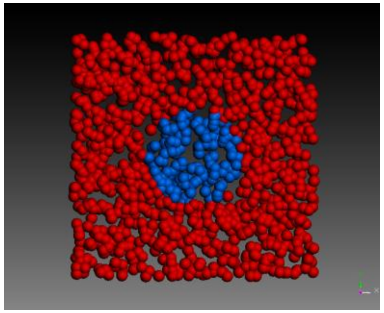
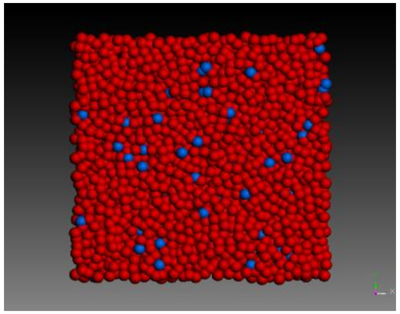
Electro-magnetic - power transfer to the walls from the induction coils

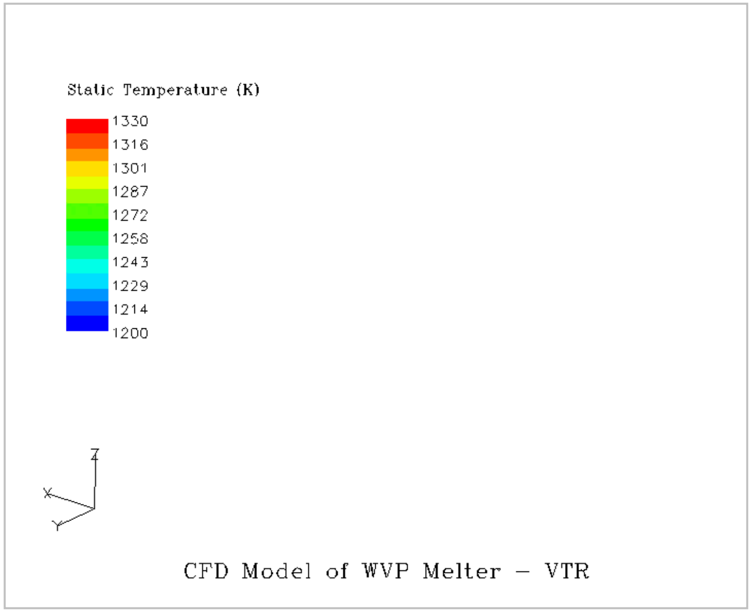




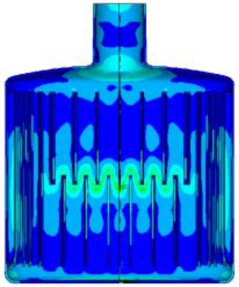
Chemical Modelling for glass physical properties







Structural stress analysis



Potential Applications
Glass Melter Analysis (1)

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- CFD/stress model of a glass melter
- Can inverse methods be used to determine the physical properties of the glass melt?
- Can the operational lifetime of the melter crucible be estimated?

Closing Remarks

- In nuclear processes measurements are taken, many systems can be simulated to an acceptable degree of accuracy
- Much uncertainty over the data input (e.g. materials and process conditions)
- The industry is heavily regulated and dealing with uncertainty and accuracy in calculations takes considerable effort
- Applications suitable for inverse methodologies exist within the nuclear industry (at least a couple of potential candidates outlined here)

Questions