

A 1D biogeochemical model framework (SMARTml) for assessing and managing acid sulfate soil risks

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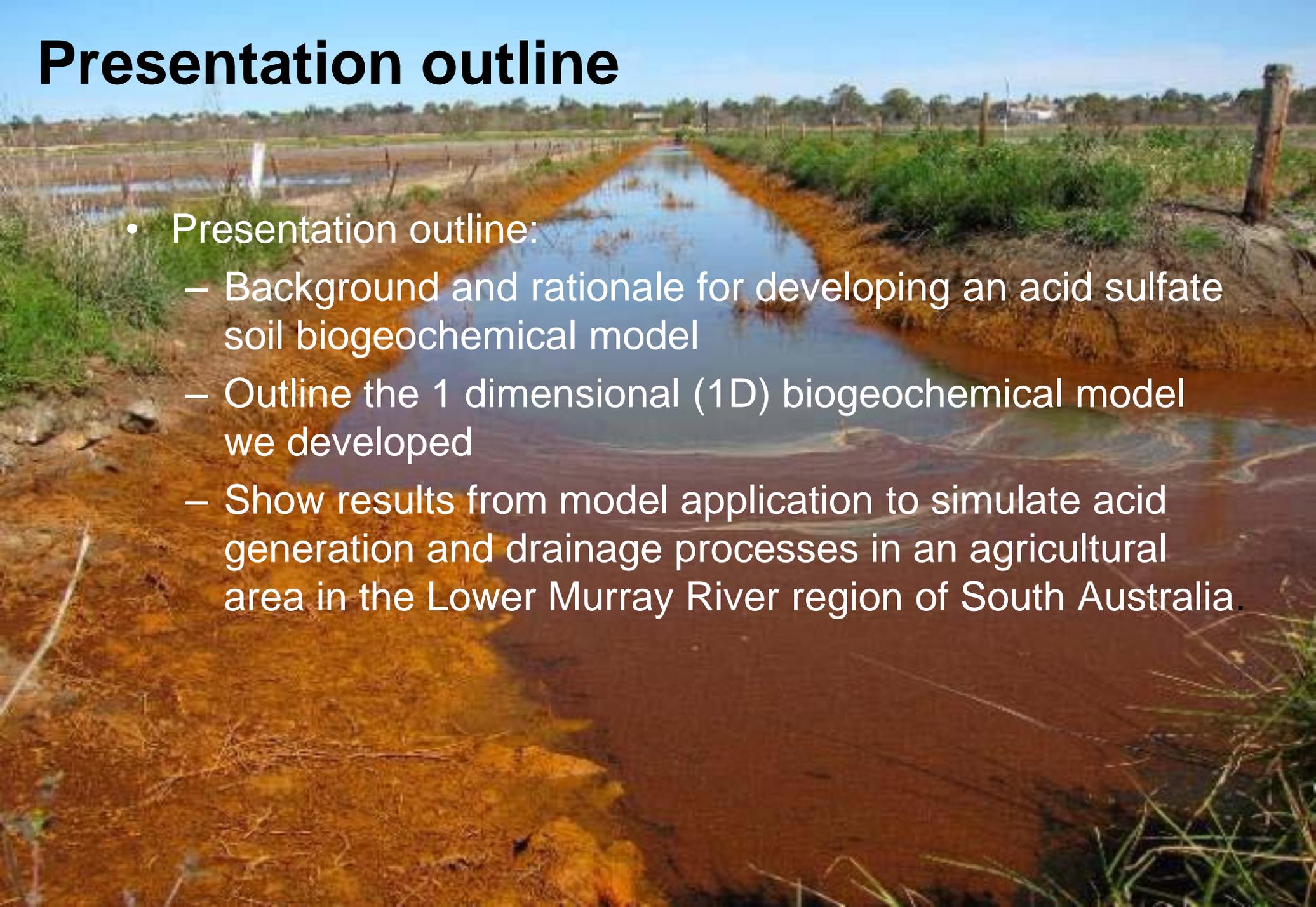
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Presentation outline

- Presentation outline:
 - Background and rationale for developing an acid sulfate soil biogeochemical model
 - Outline the 1 dimensional (1D) biogeochemical model we developed
 - Show results from model application to simulate acid generation and drainage processes in an agricultural area in the Lower Murray River region of South Australia.



Background

- Acid sulfate soils and acid mine drainage poses significant management challenges and risks to the environment
- Application of modelling to ASS has been limited (Bronswijk, Groenenberg et al. 1992/1993) although some mining-based pyrite oxidation models exist (Wunderly et al 1996)
- Complex biogeochemical modelling problem involving oxygen transport into the sediment, kinetic reactions (e.g. pyrite oxidation), secondary mineral formation/dissolution, mineral:solution equilibria, transport processes, acid neutralisation reactions.



Why model acid sulfate soils?

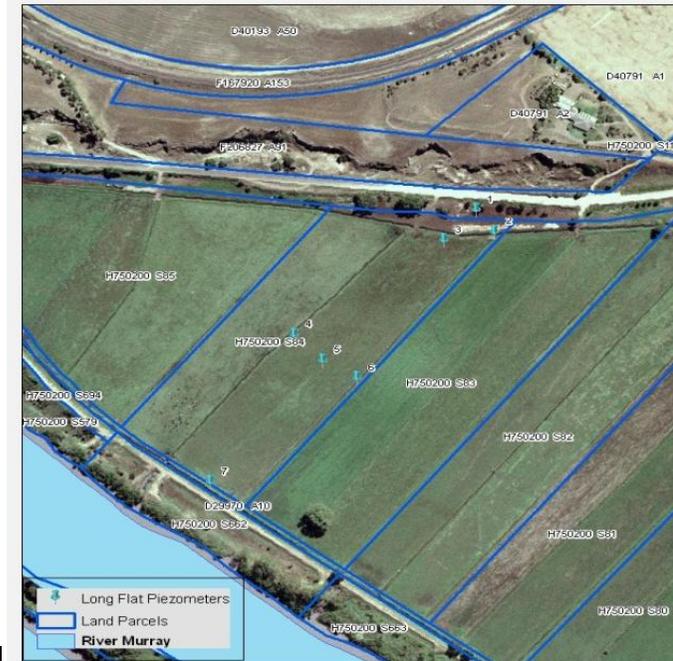
- Geochemical modeling could potentially be very useful in predicting and managing ASS impacts (e.g. oxidation given particular hydrology, metal release and export, recovery timescales).
- Management actions are, and must, be taken regardless if a model is used.
- We know that all modelling of natural processes is inaccurate to some degree and models do not include or adequately represent all biogeochemical processes (e.g. assumption of equilibria, simplified abstractions of nature). Should we not bother?
- Zhu and Anderson (2002)¹ state *“The question really is whether the model results are useful, and more useful than not modelling at all, or modelling with methods that are known to be less accurate than other methods. We believe that modelling is part of the essence of science; that field or analytical data must be brought together in a framework. Carrying out modelling always results in increased insight into the problems involved.”*
- Power of a (good) model is that it enables prediction of future conditions

¹ Zhu and Anderson (2002) Environmental Applications of Geochemical Modelling. Cambridge University Press, 284pp.

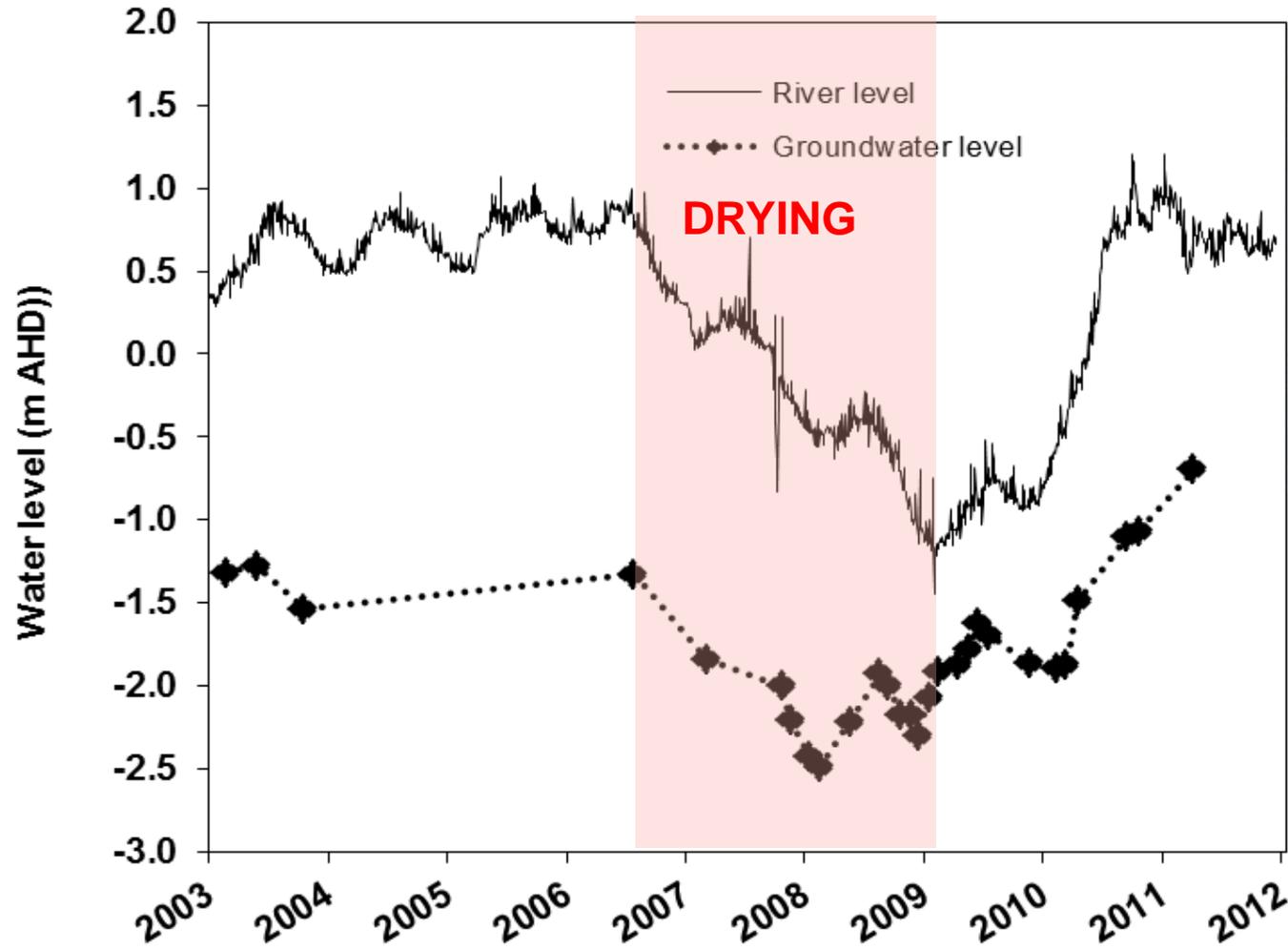
Site and data for modelling

- River water levels, long term groundwater levels
- Trial site intensively monitored over 18 months to collect data for model
- Multi-level piezometers – pH, salinity, redox potential, acidity/alkalinity, metals, major ions, DOC
- Soil cores – acid base accounting (pyrite, retained acidity, available acidity, ANC), metal sequential extraction, exchangeable cations, organic matter, mineralogy, particle size (% sand, silt, clay), pyrite crystal size

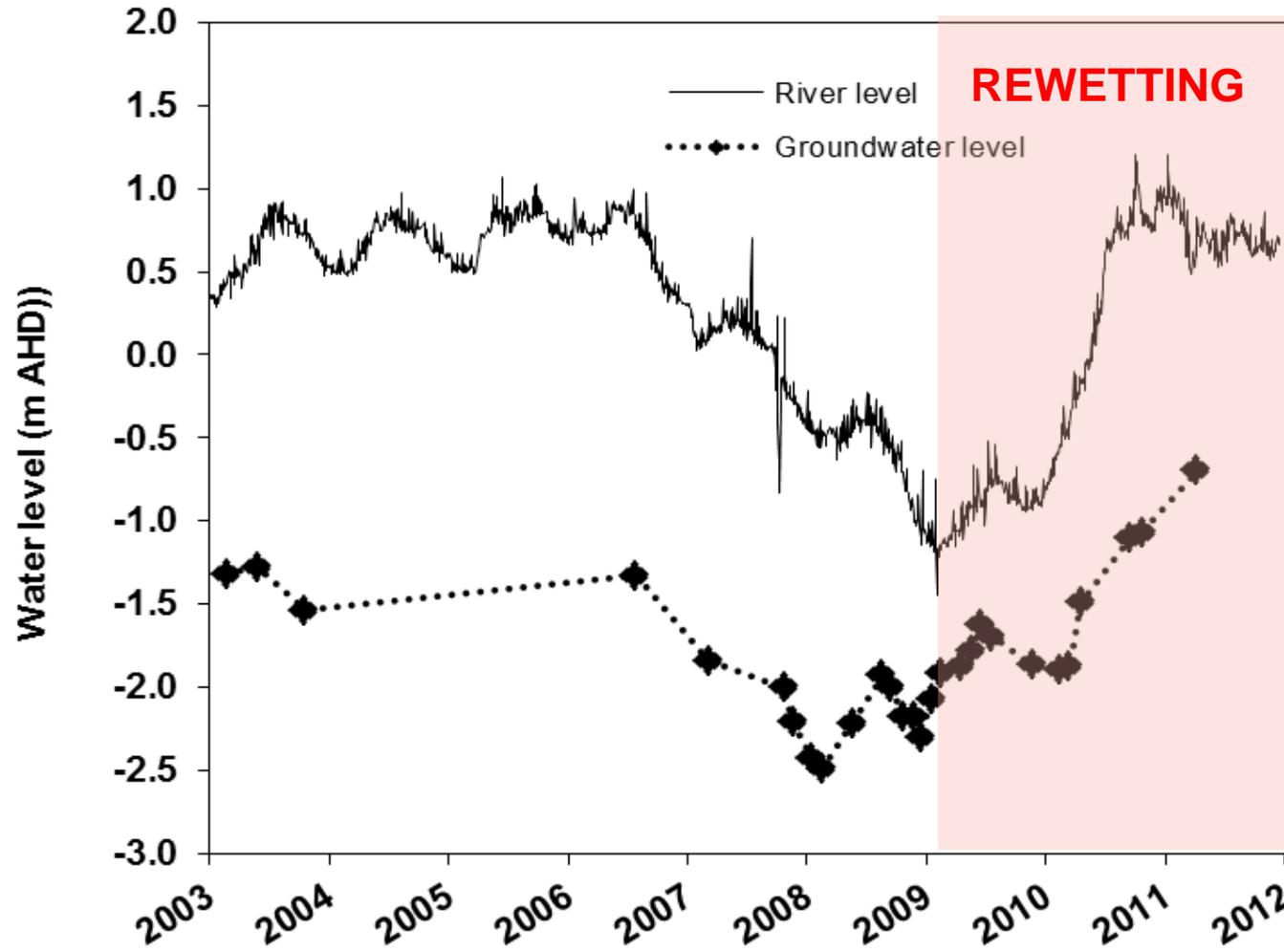
Long Flat Piezometer Location



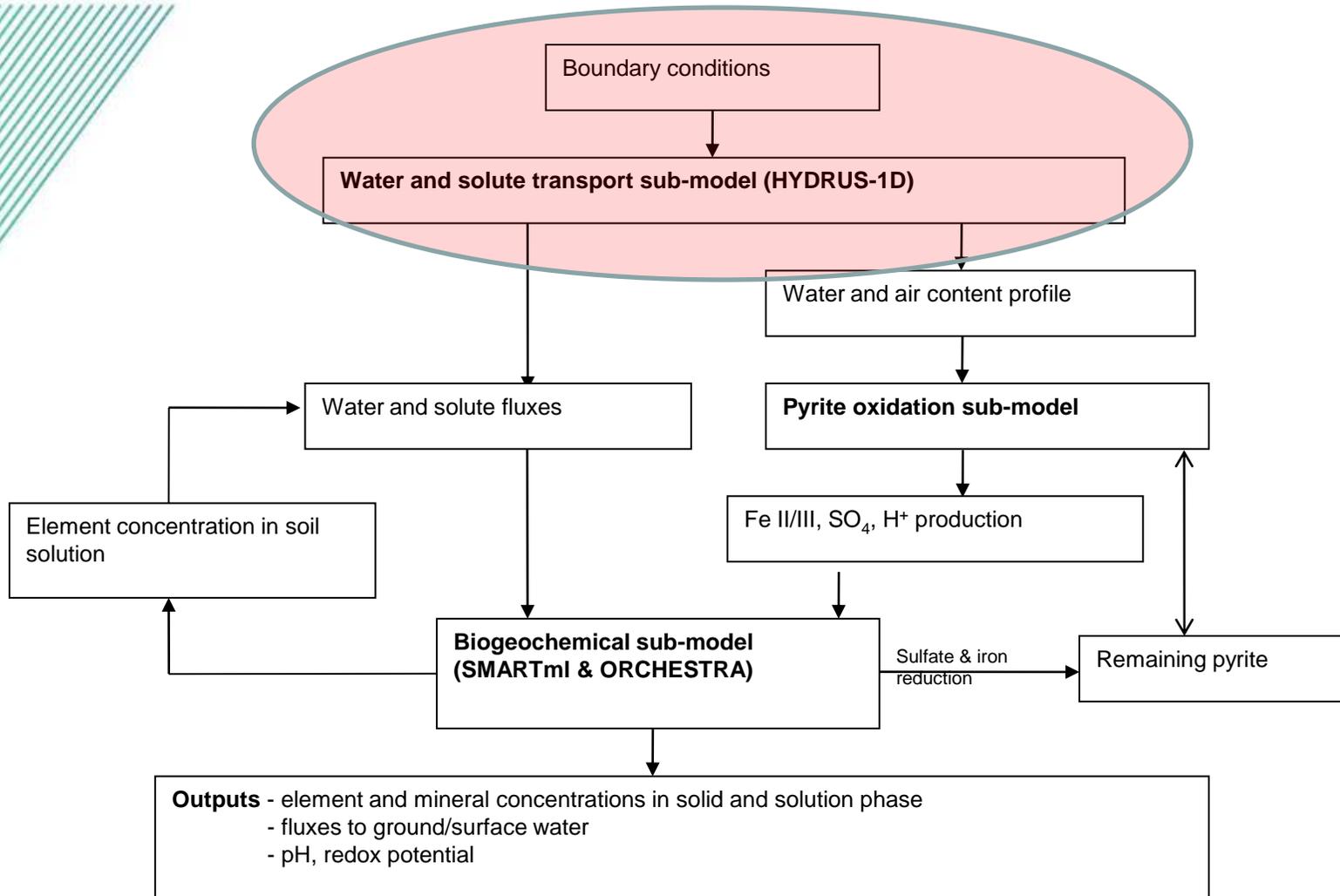
Associated groundwater decline



Associated groundwater decline

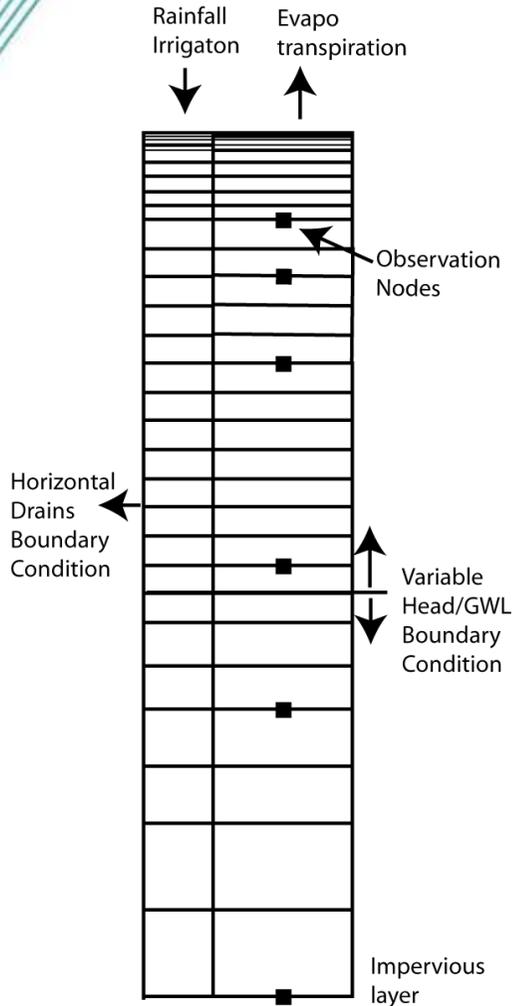


Overview of model - hydrology

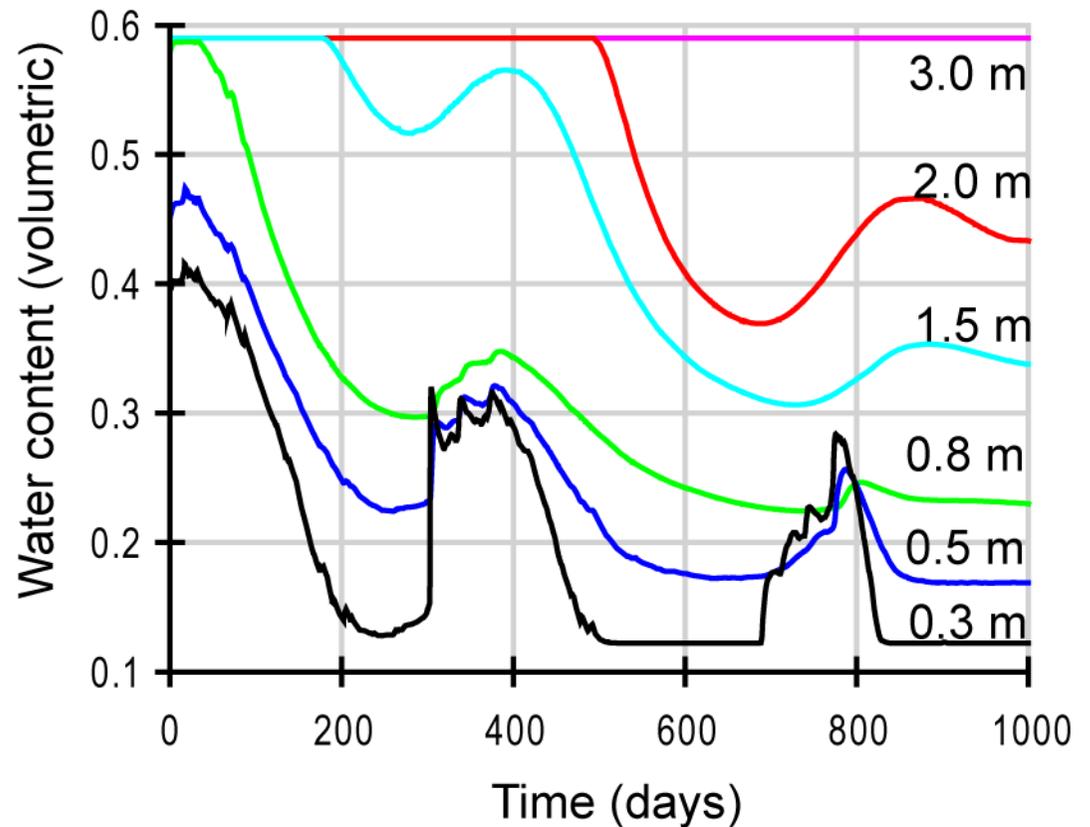


Hydrus 1D public domain model for water and solute flows in variably saturated soils. Windows based with graphical user interface

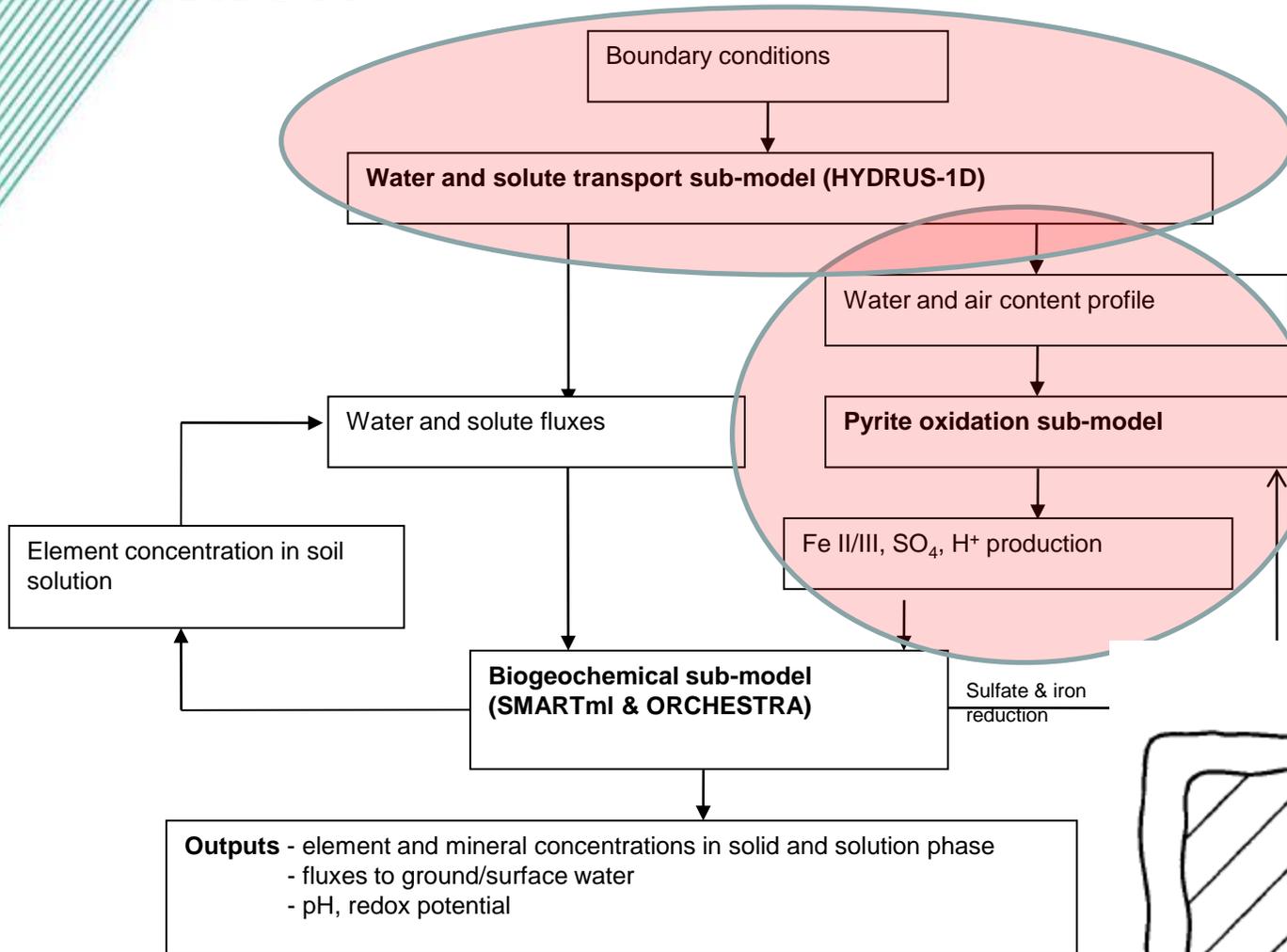
Hydrus setup and key output



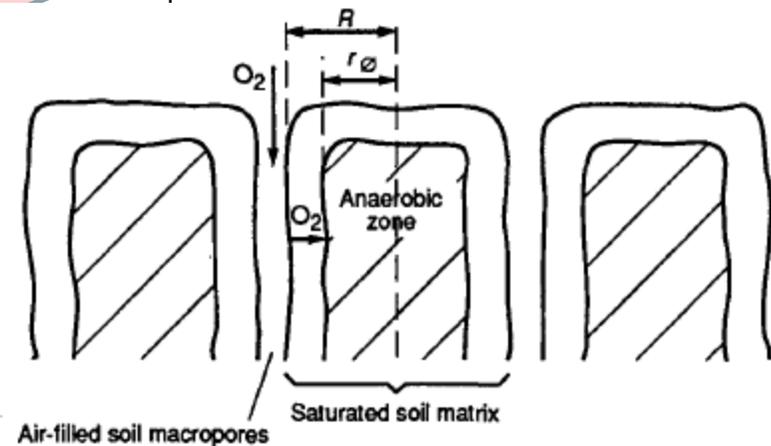
Observation Nodes: Water Content



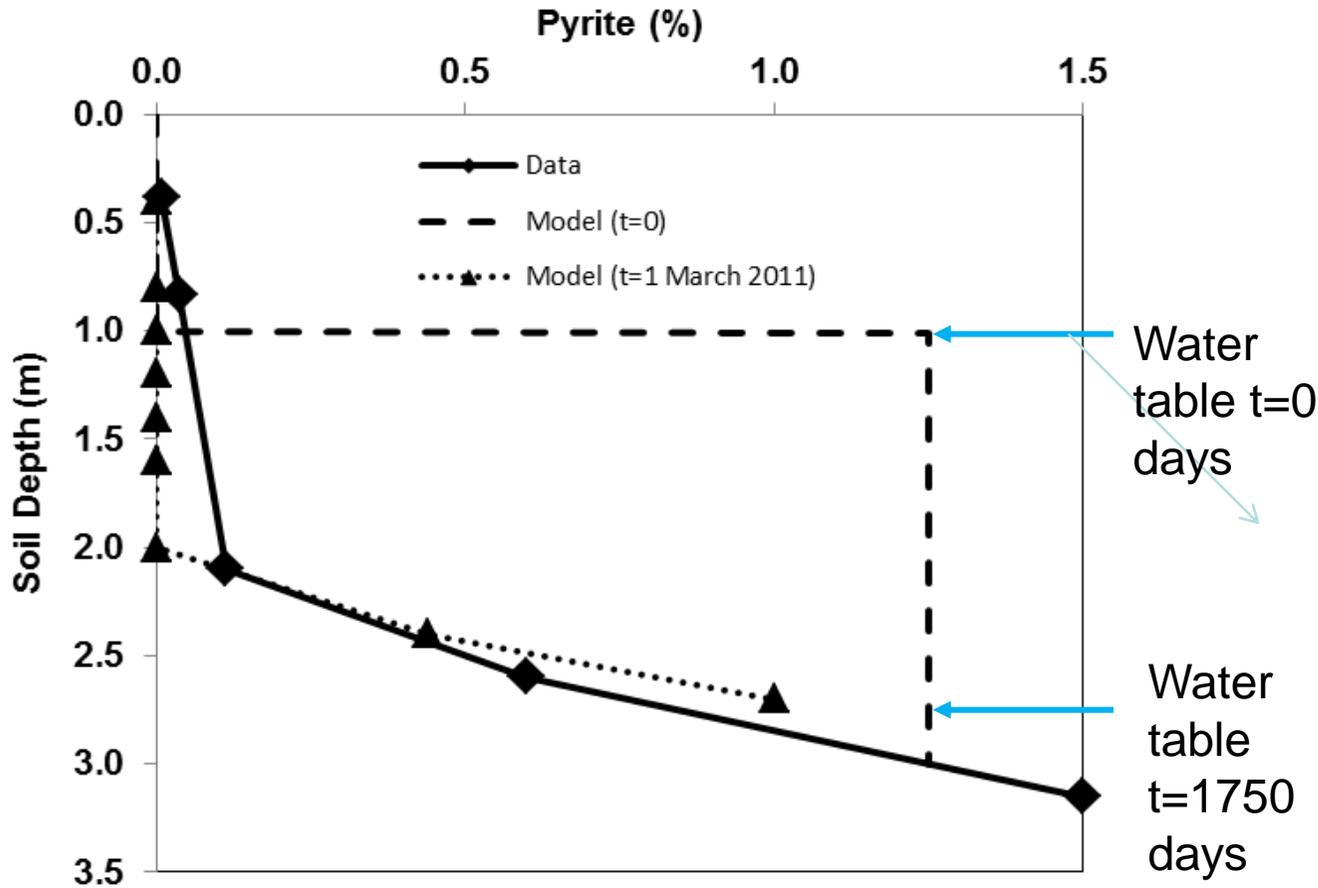
Overview of model – pyrite oxidation



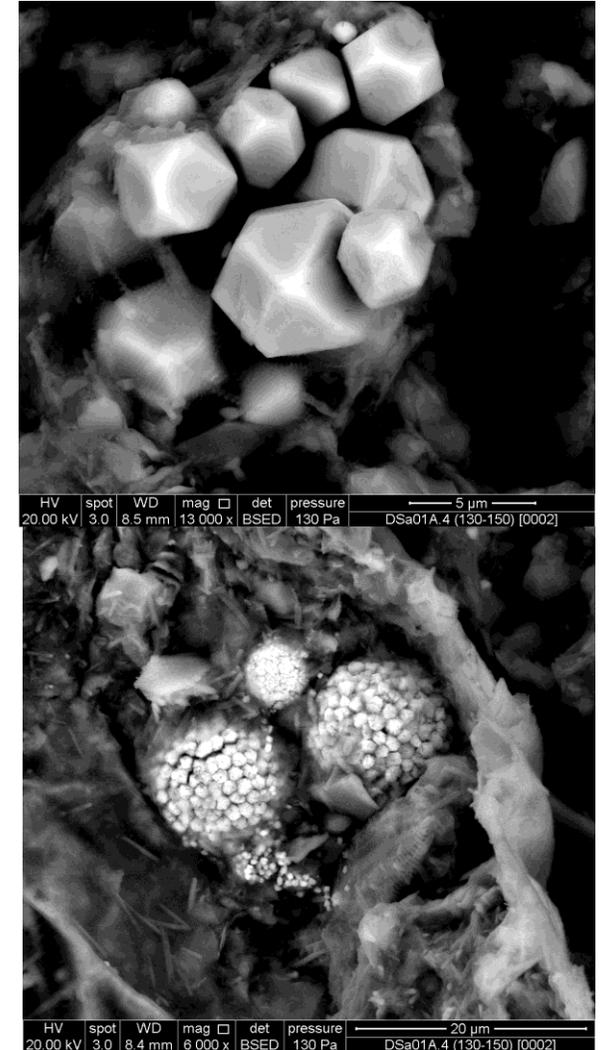
Pyrite oxidation model based on published work by Bronswijk, Groenenberg et al. (1992, 1993, SMASS model). Oxygen diffusion through macropores & aggregates, pyrite-organic matter competition for O₂, pyrite crystal size/diameter (shrinking core model)



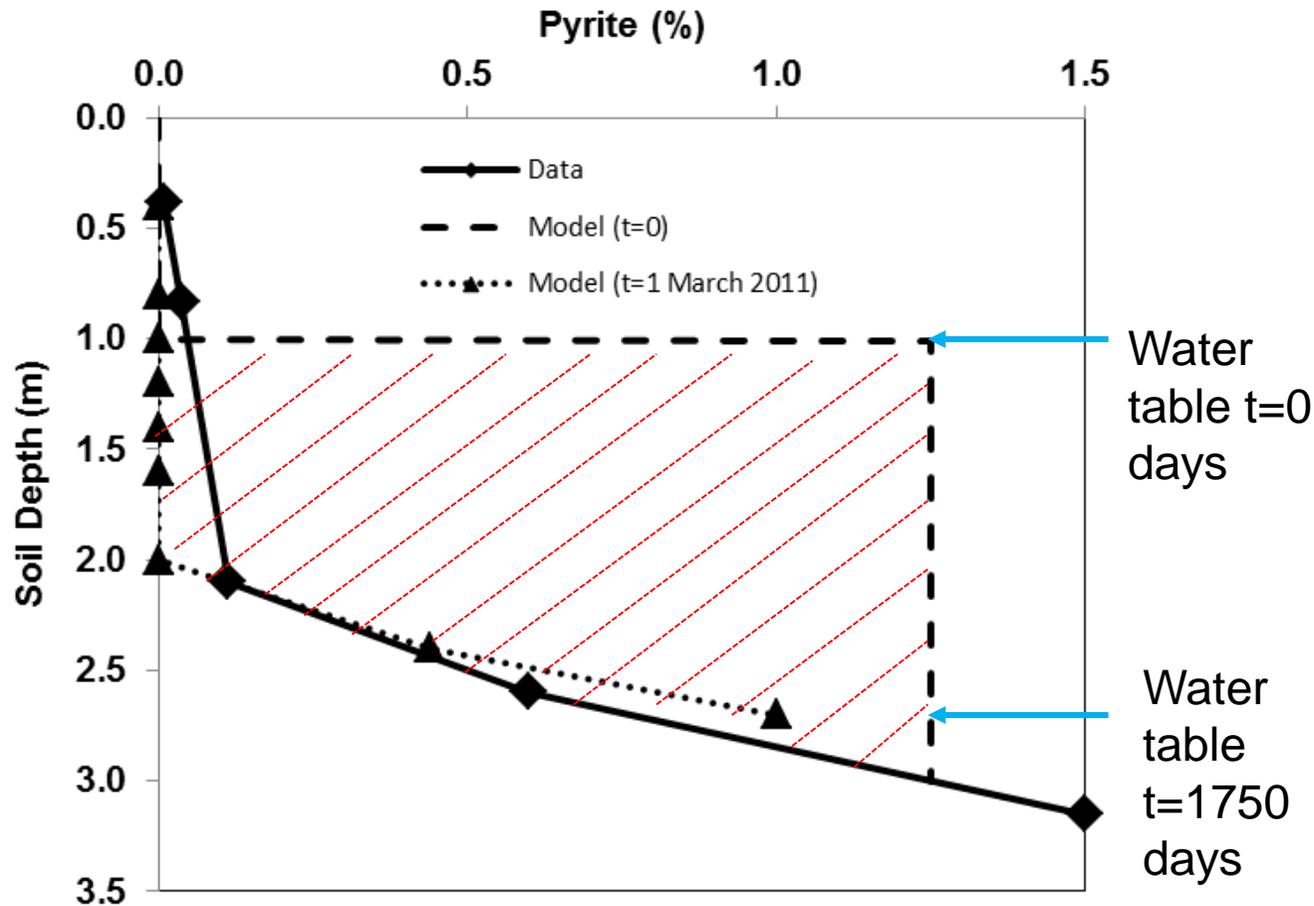
Modelled vs measured pyrite oxidation



5 year simulation (day 1705 in model)

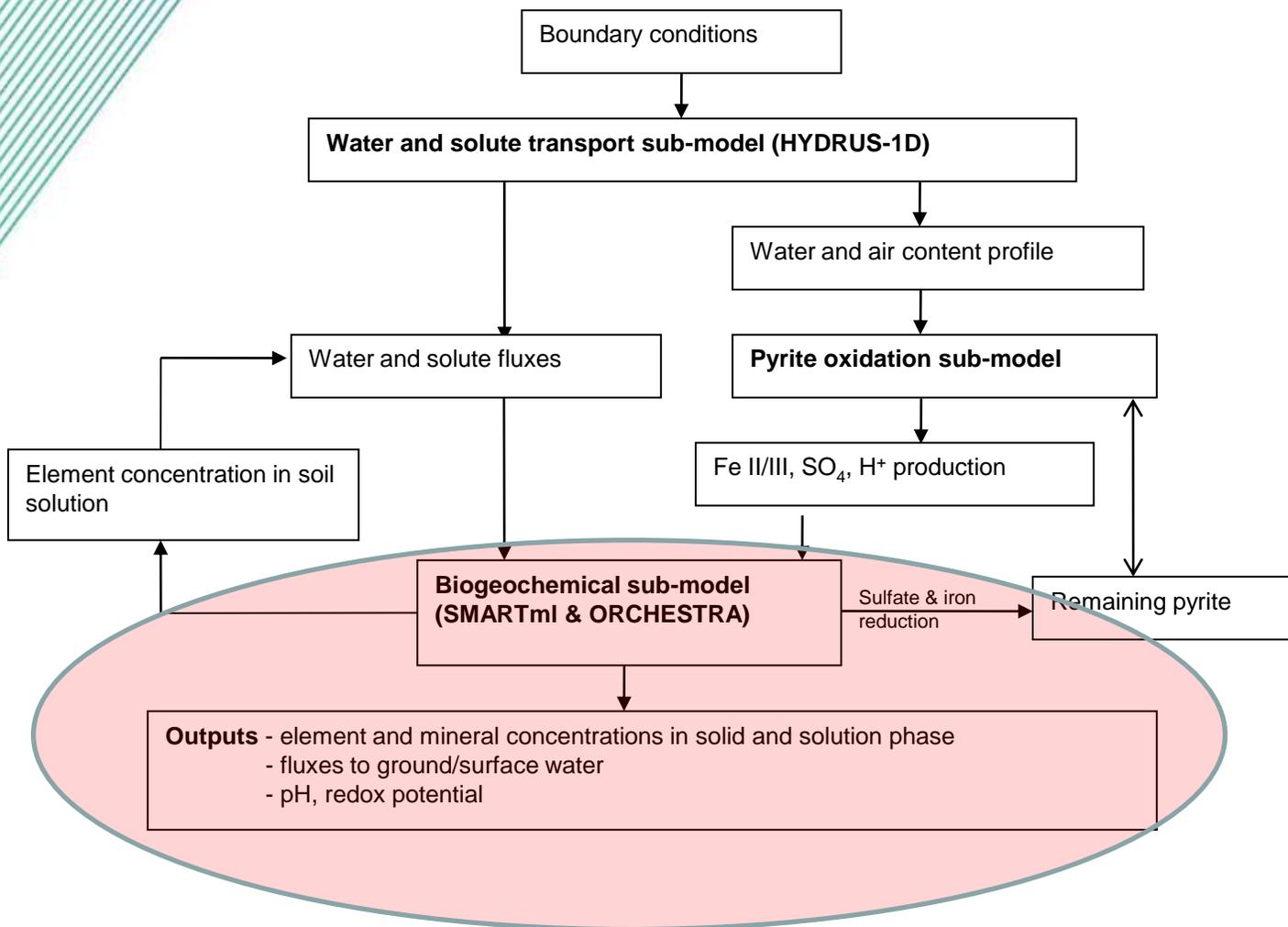


Modelled vs measured pyrite oxidation



5 year simulation (day 1705 in model)

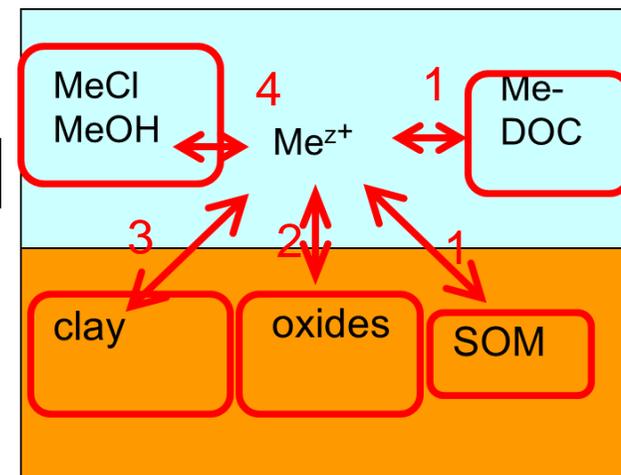
Overview of model



Other reactions included in SMARTml (kinetic) - ORCHESTRA (equilibria) biogeochemical model (Bonten et al. 2011). Includes metal binding to multi-surfaces – clays, oxides & organic matter,

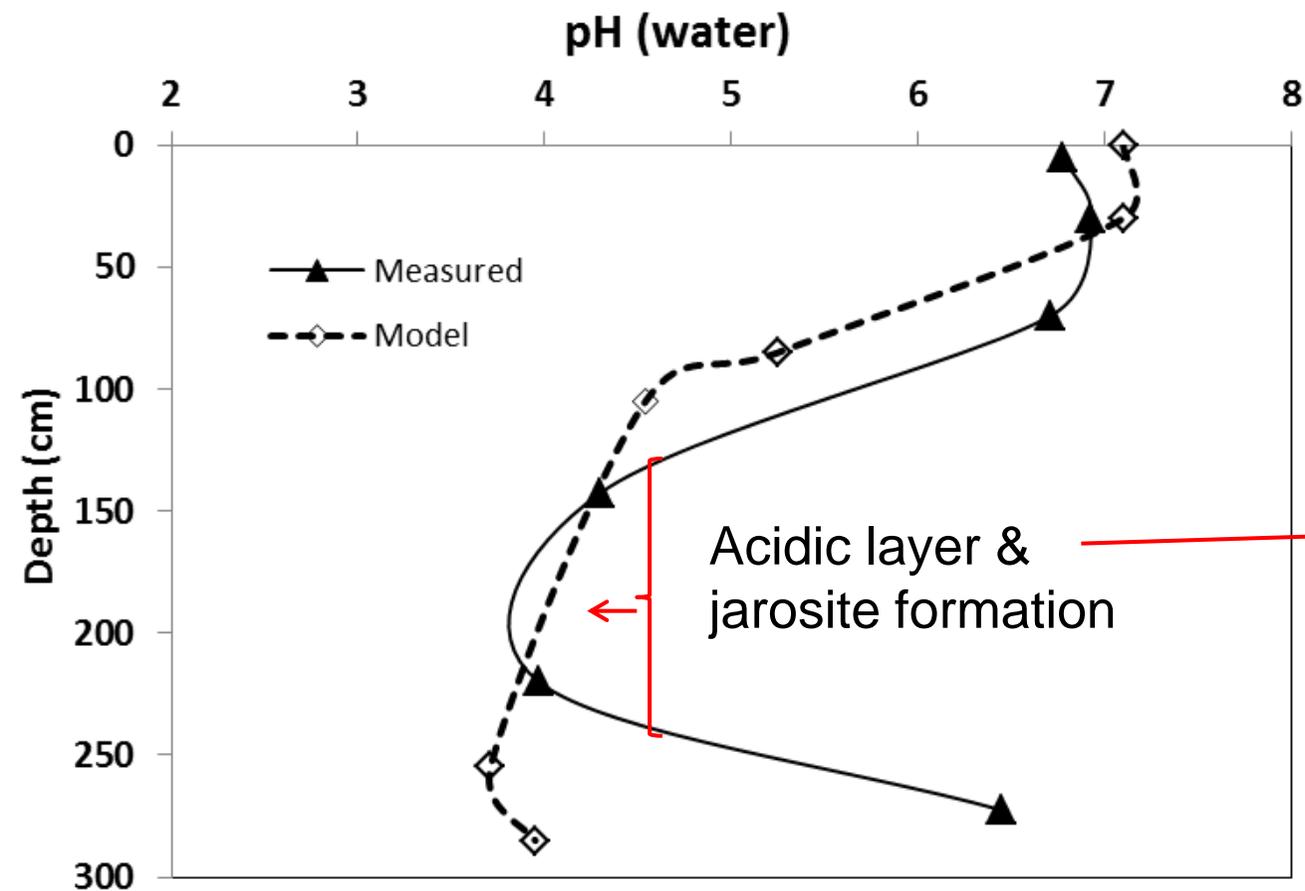
Jarosite, Fe(OH)₃, Al(OH)₃ precipitation/dissolution

Sulfate and iron reduction.



1 Nica-Donnan 3 Donnan
2 GTLM 4 Minteq

Soil acidity formation



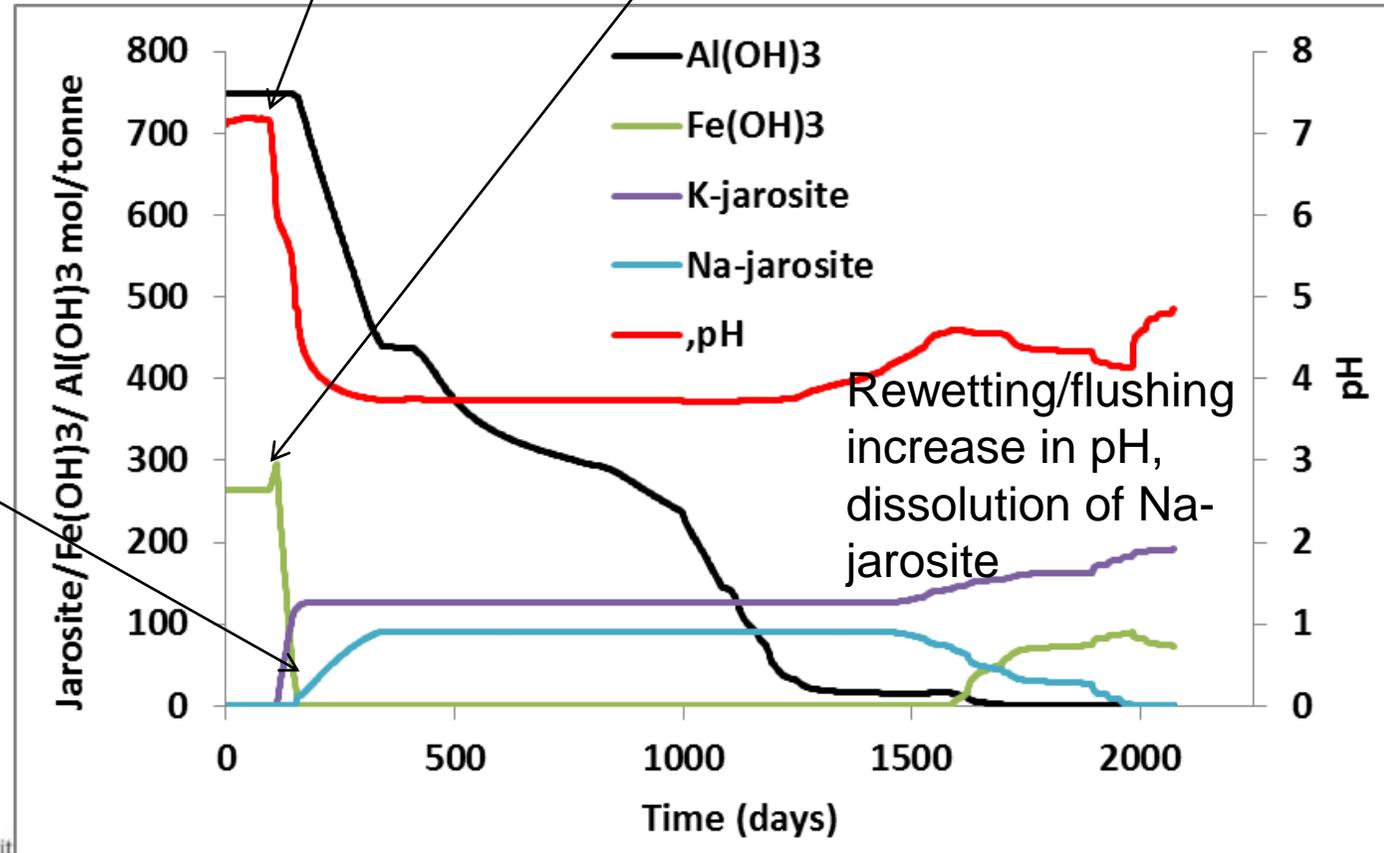
Geochemical processes



pH initially buffered by cation exchange then $\text{Al}(\text{OH})_3$.

Ferric (III) oxide formed following pyrite oxidation and then dissolved as pH lowers

K- and Na-jarosite is formed at the expense of Ferric (III) oxide. However the formation of Jarosite is limited by the amount of K and Na in the soil



Predicted vs observed metal concentrations

Model inputs (measured)

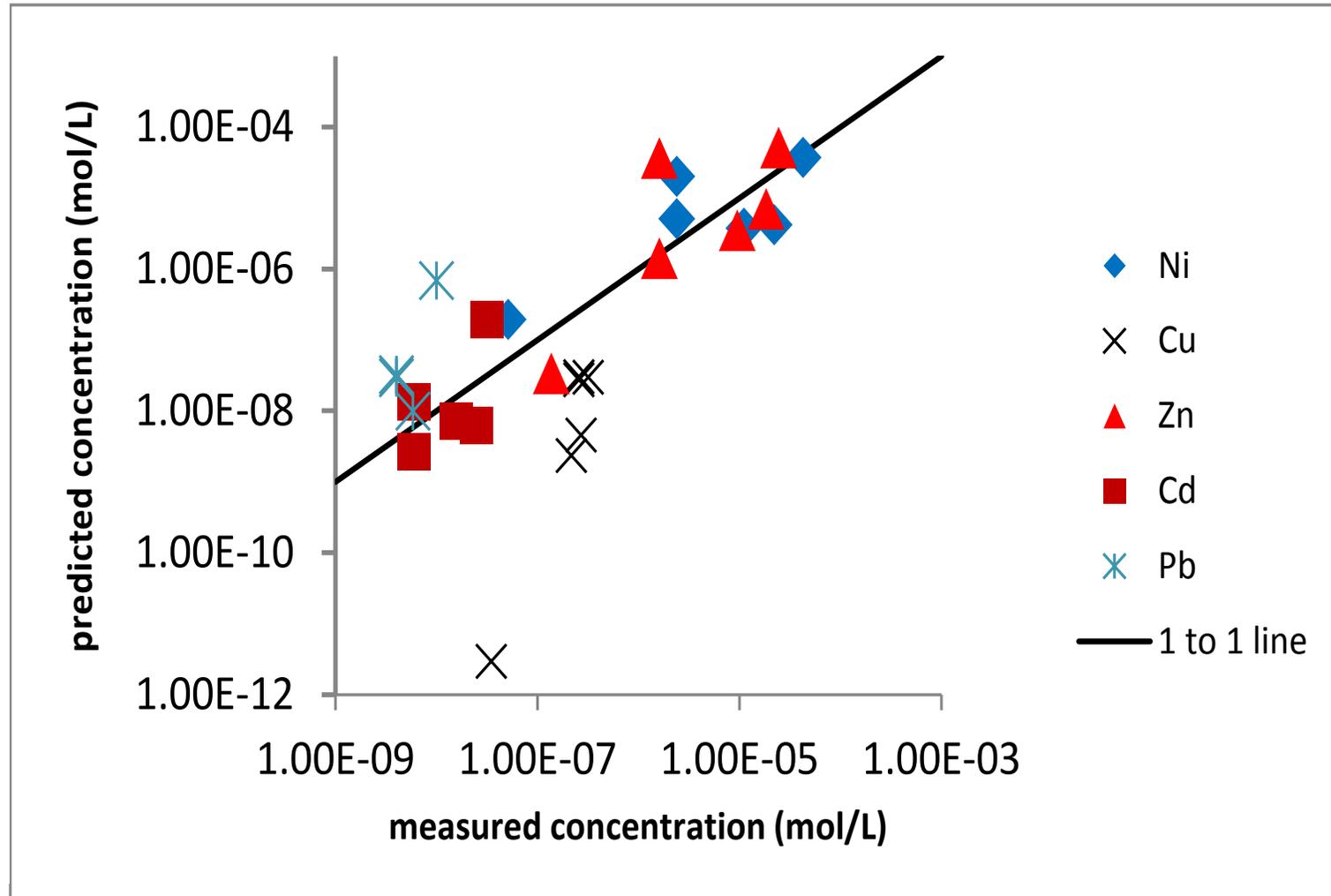
Soil reactive metal content
-selective extraction (1M
MgCl₂+1M HCl)

Soil Al + Fe oxides
(selective extraction 1
MHCl + pyrophosphate)

Soil organic matter - 50%
reactive (humics)

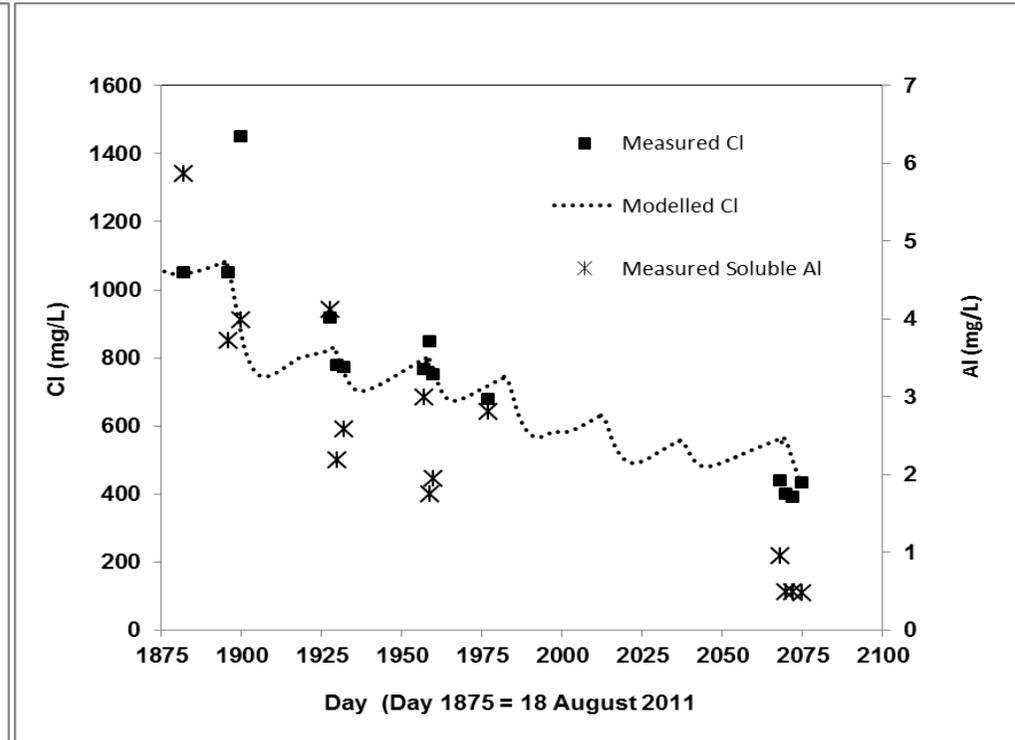
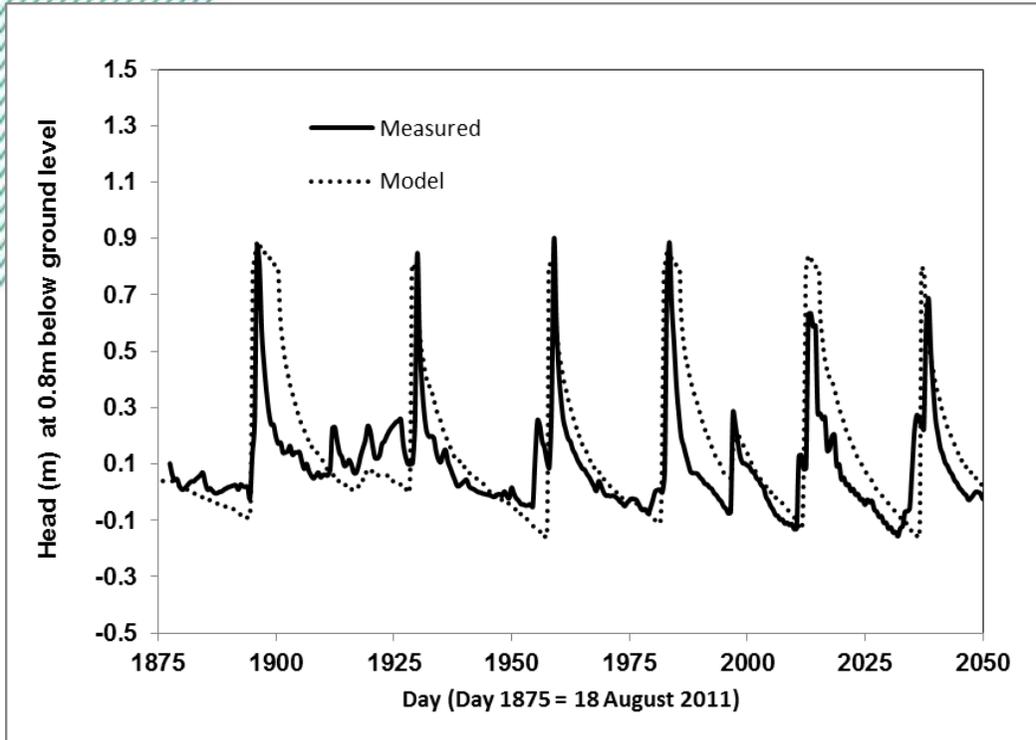
DOC in solution - 50%
reactive (humics, fulvics)

pH and major ions in
solution



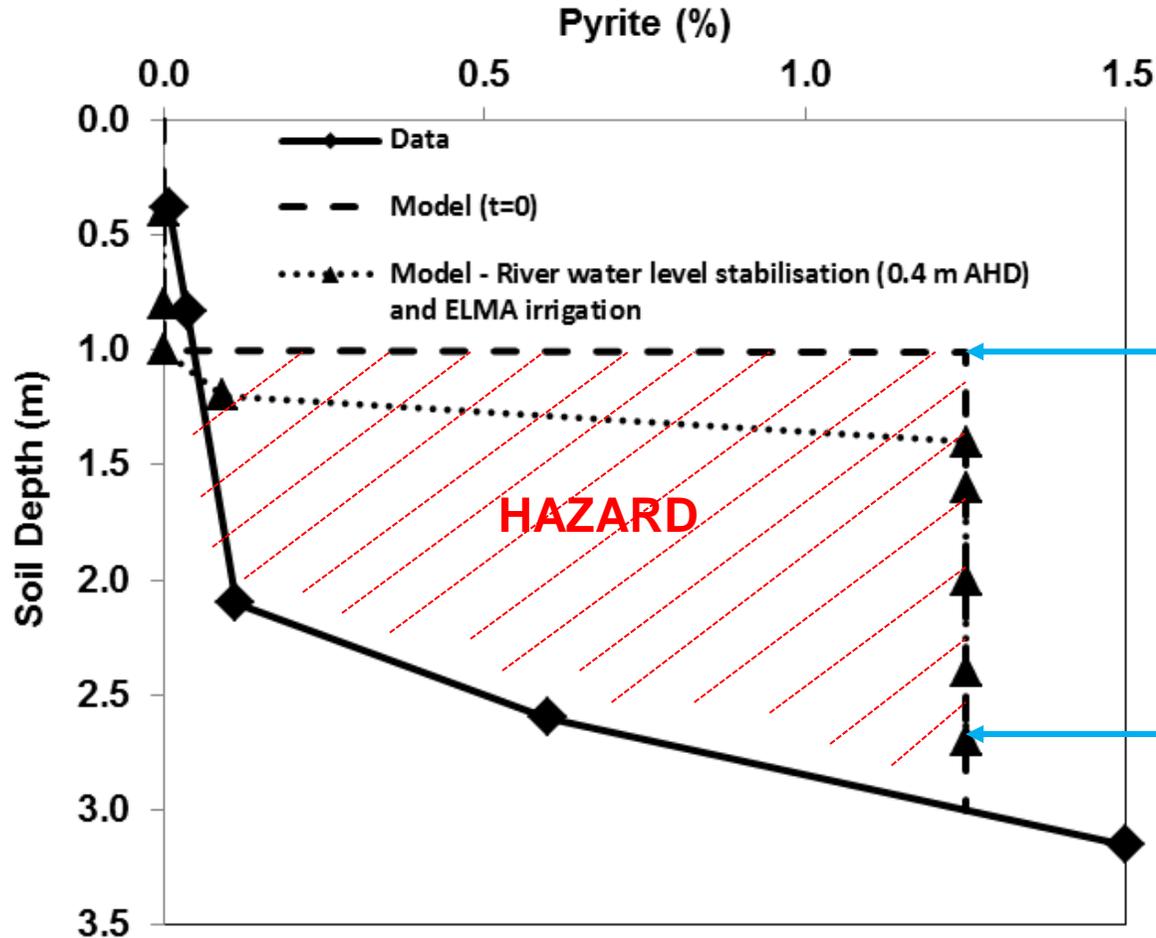
Predicted equilibrium concentrations in solution based on present metal contents in soil

Flushing with irrigation



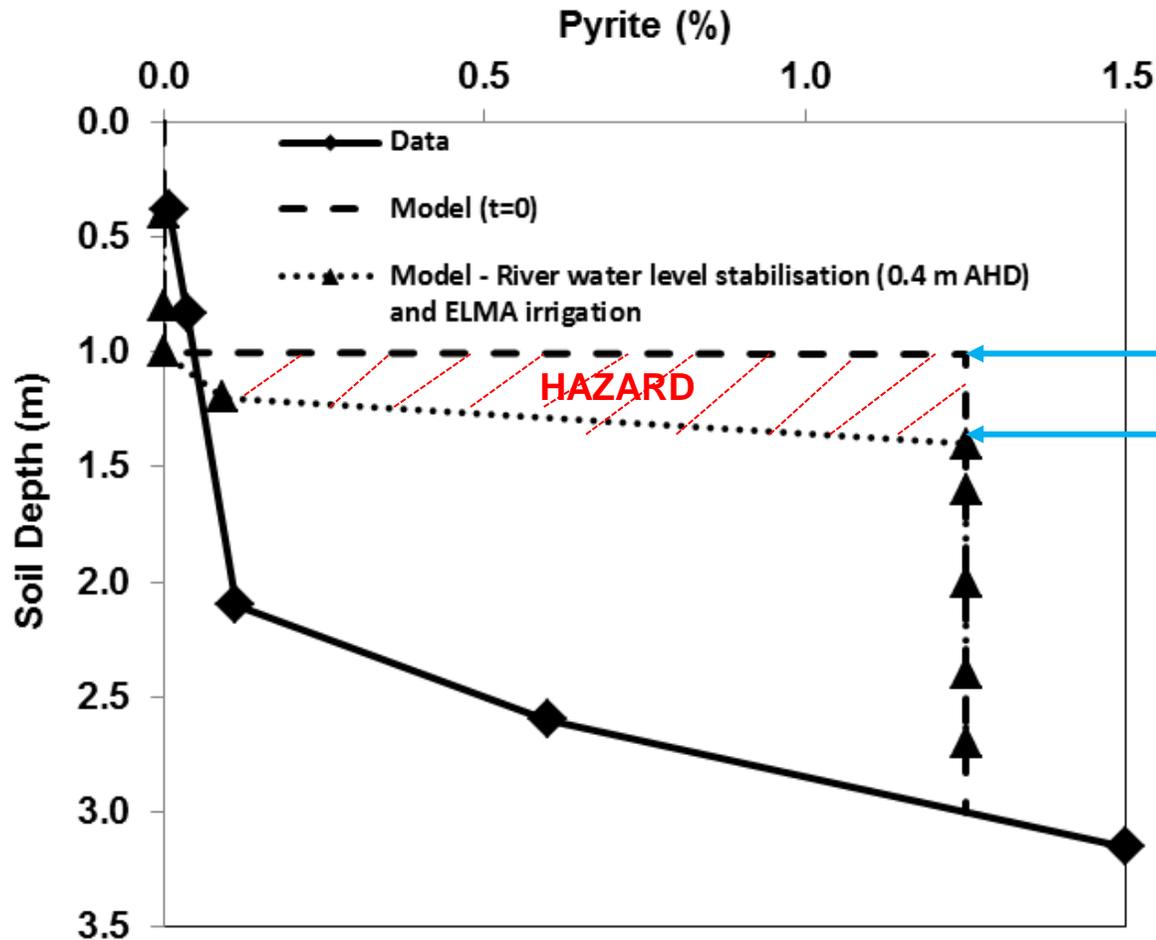
Mid level piezometer data (screened -0.75 to -1.25m below ground level)

Management scenario



River and ground water level decline resulting in large zone of pyrite oxidation = LARGE HAZARD

Management scenario



Groundwater level decline and pyrite oxidation minimised (river level falling <0.5 m and 2 'environmental' irrigations per year) = MUCH SMALLER HAZARD

Summary

- New 1D biogeochemical model developed to assess and manage acid sulfate soils
- Successfully represented pyrite oxidation, acidity generation, and solution metal concentration in a 3m deep soil profile over a 6 year simulation
- Model proved useful, increased our insight into processes, delivered management outcomes

Acknowledgements

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- Emily Leyden and David Palmer (EPA) for field assistance
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