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Modelling of ion exchange for water treatment in the nuclear industry...

...using high performance computing and custom web interfaces for large scale sensitivity studies

Steve Baker & Jonathan Austin

What is NNL

- The National Nuclear Laboratory (NNL) was formed from the Research and Technology organisation of BNFL
- Currently operates as a Government Owned Contractor Operated company which
  - Employs 800 people
  - Operates 6 active and non-active facilities
  - Has a turnover of £84M
- Customer base across the nuclear industry including
  - Sellafield Limited
  - Nuclear Decommissioning Authority
  - Magnox Electric
  - EDF
  - MOD

History of Modelling in NNL

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- Modelling goes back to the start of the nuclear industry and covers a wide range of disciplines
- Current team Chemical and Process modelling has a continuous history back to the early 1980's
- Team size usually in the range 10-15 Engineers/scientists
- Modelled most unit operations including
  - Solvent extraction
  - Filtration
  - Ion Exchange
  - Distillation
  - Evaporation

History of Modelling in NNL

- For many reasons
  - Flowsheeting/design support
  - Process Development
  - Process Control
  - Plant optimisation
  - Safety/environmental cases

History of Modelling in NNL

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- Tools used (as this is a user conference)
  - Fortran
  - SpeedUp
  - ACM
  - gPROMS
- Plus a range of chemical modelling tools including
  - PHREEQC (speciation modelling)
  - Quantum Mechanics
  - Molecular Dynamics
- Close links to other modelling areas
  - CFD Fluent/CFX

What is SIXEP?

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Site Ion eXchange Effluent Plant

SIXEP - Design Specifications

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- SIXEP is a Low Activity Effluent Treatment Plant implementing Ion Exchange technology.

- It uses Best Practicable Means (BPM) for removing:
  - - Suspended solids (associated alpha-activity)
  - - Soluble caesium (beta-activity)
  - - Soluble strontium (beta-activity)

- Operational since 1985.

- SIXEP capacity is 4200 m^3/day.

- Designed to be operational for 30 years.

Goals of SIXEP

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- Effective reduction of the activity in the effluent streams discharged to the environment.
- Production of stable secondary radioactive waste.
- Low volumes of secondary waste formed.
- Robust System:
  - Deals with waste from a number of different sources
- SIXEP has been a tremendous success for the Sellafield site

Reduction in Alpha and Beta activity to Sea

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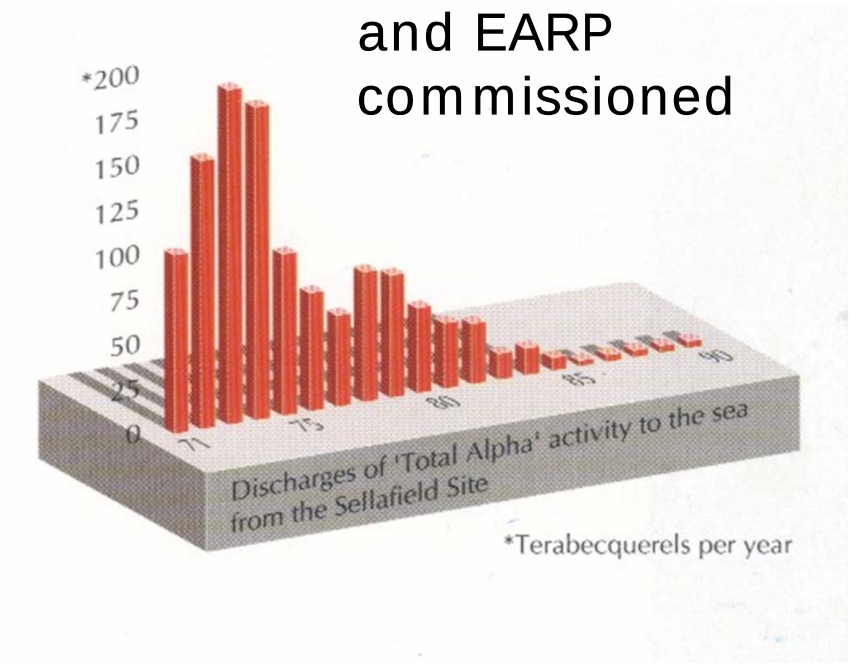
1985: SIXEP and EARP commissioned



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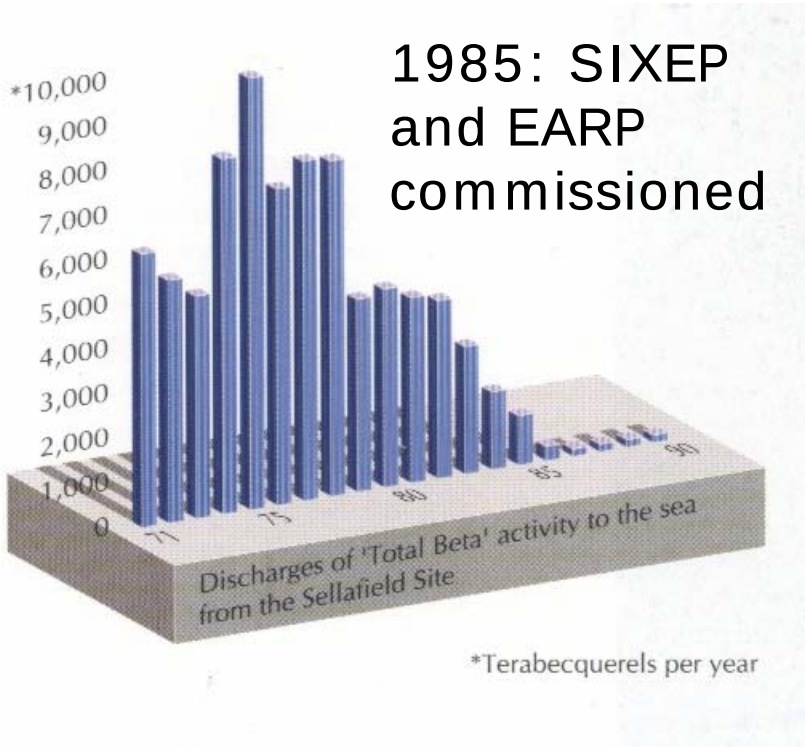

The problem

- SIXEP was designed 30+ years ago for a particular type of effluent
- Sellafield effluents are changing as site is remediated
- Expectation is for continuing high performance
- Life is being extended to potentially 70 years

What we need to do

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- Develop a tool to predict plant output over the next 4 decades
- Preserve the life of the ion exchange beds
- Prevent out of spec discharge to the environment
- Analyse proposed feeds to plant

How we are going to solve it

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- Production of a process & chemistry model
- Supported by experimental work
- Validated against plant feed and discharge data
- Implemented through a web interface

SIXEP schematic

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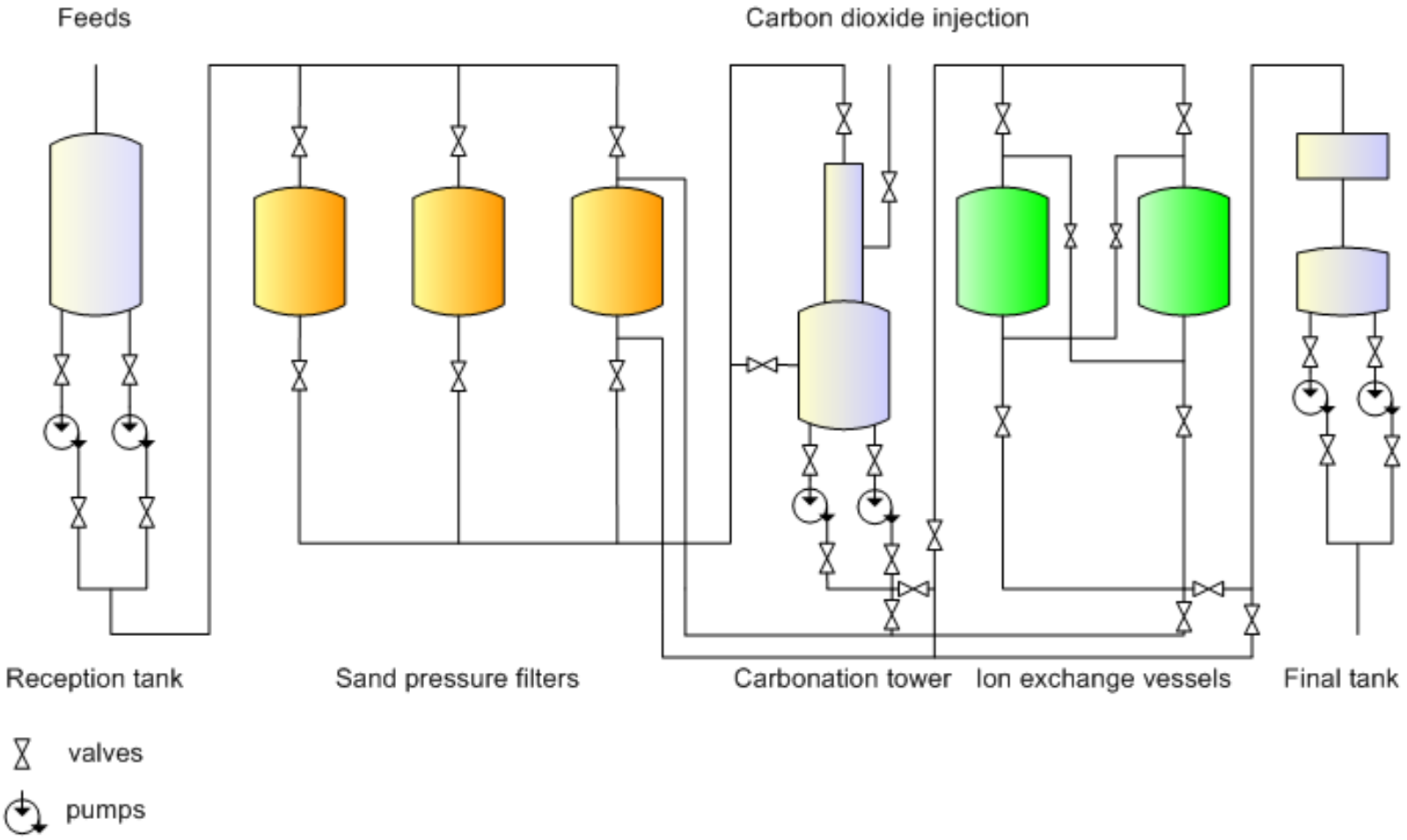

gPROMS Model

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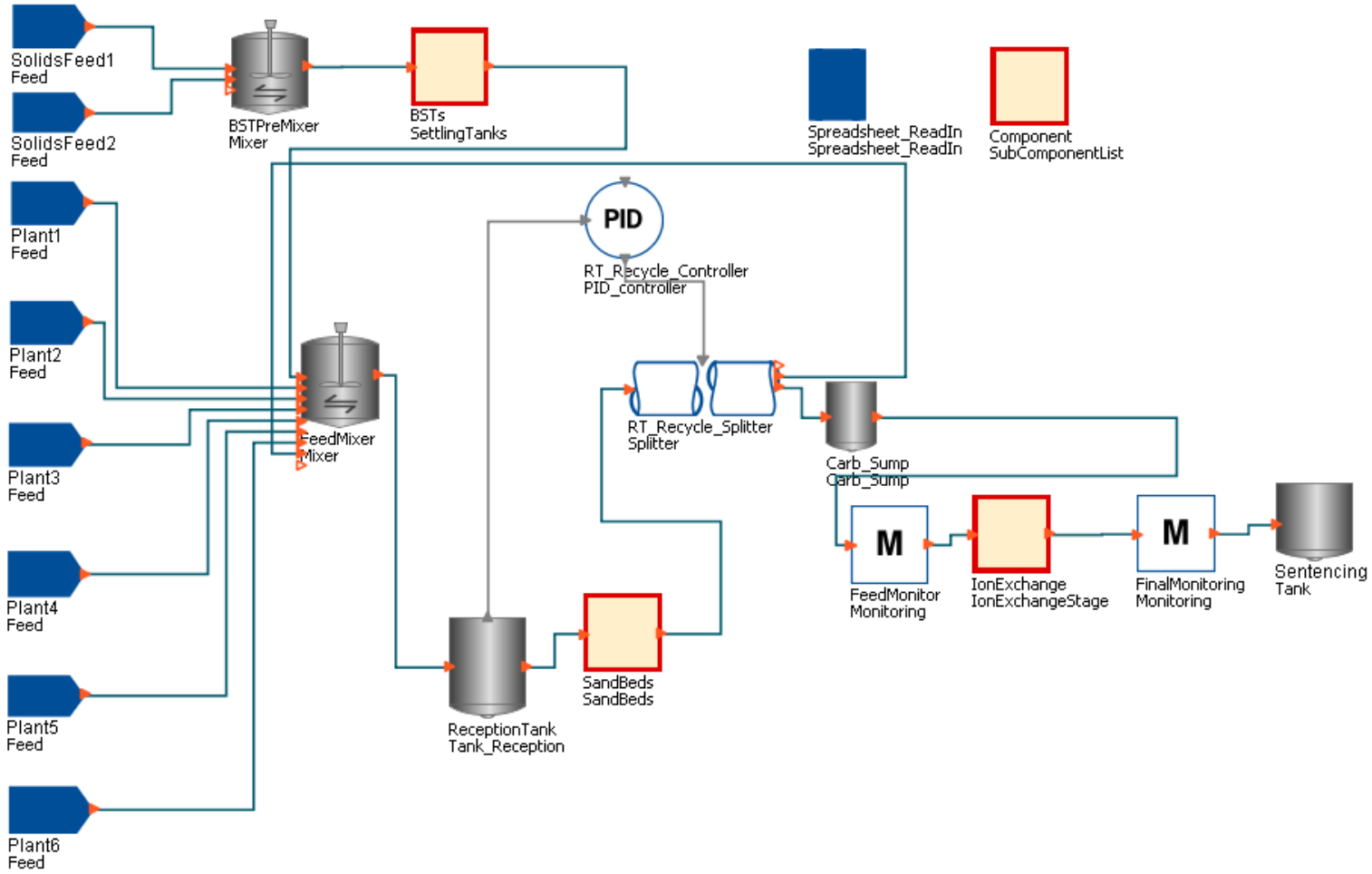

gPROMS Model

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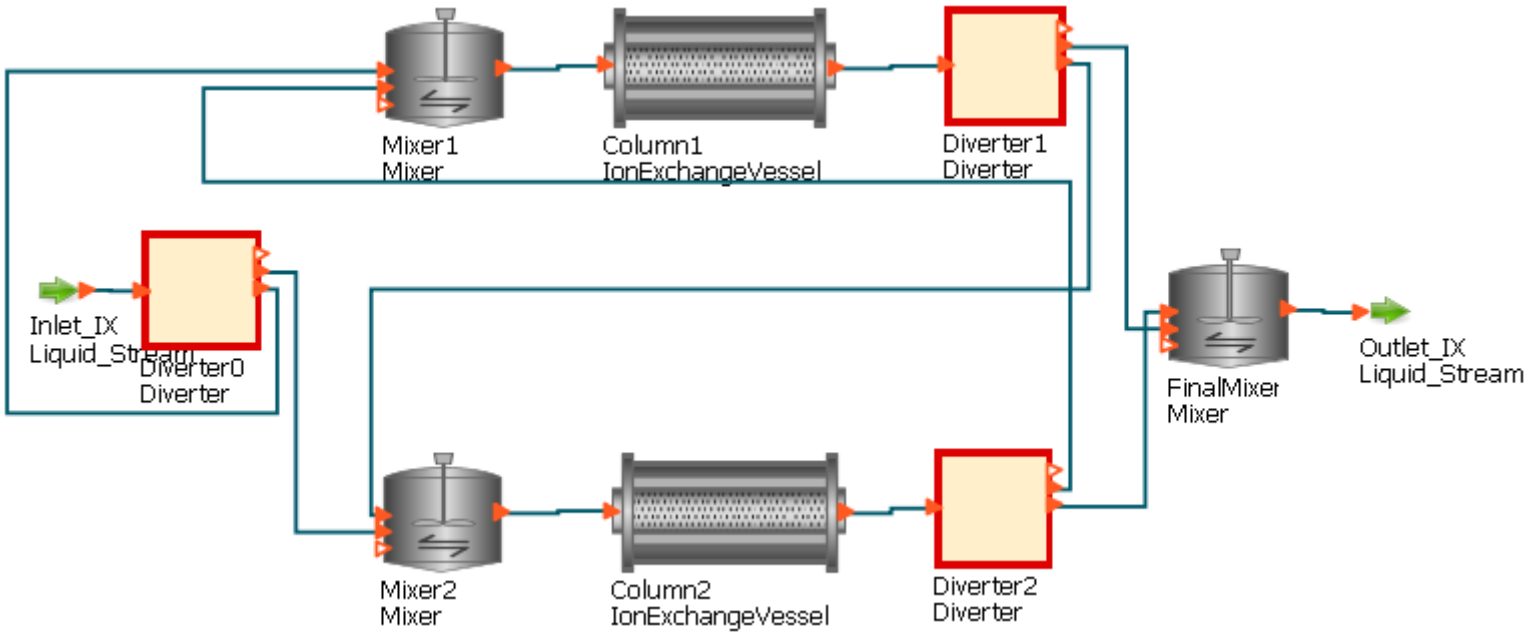

Ion Exchange Material

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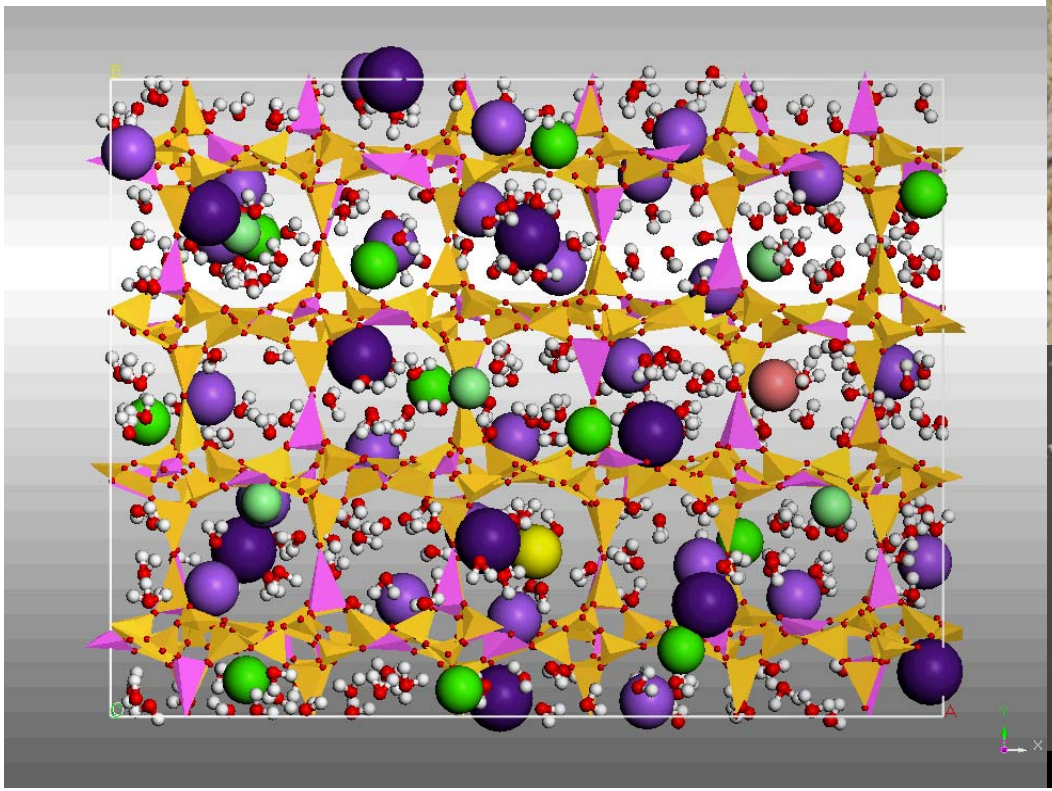
- Natural Zeolite material (strong):
  - Molecular sieve
  - Cation-exchange



Knowledge Capture

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- IX column trials
- Sand bed rig trials
- Plant sampling
- Fundamental understanding
  - Molecular dynamics
  - PHREEQC

Experiment → Modelling → Plant Consequence

Dynamic Ion Exchange Reactions

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- Ion exchange follows a reversible mechanism:
  - $Na^{+}_{ex} + Cs^{+}_{aq} \Leftrightarrow Na^{+}_{aq} + Cs^{+}_{ex}$
  - $2Na^{+}_{ex} + Sr^{2+}_{aq} \Leftrightarrow 2Na^{+}_{aq} + Sr^{2+}_{ex}$

- Ion exchange efficiency for Cs^{+} and Sr^{2+} is affected by:
  - Rate of reactions
  - Concentrations of competing cations
  - Flow rate
  - pH
  - Speciation

$$mA^{n+}_{ex} + nB^{m+}_{aq} \Leftrightarrow mA^{n+}_{aq} + nB^{m+}_{ex}$$

What can the model do?

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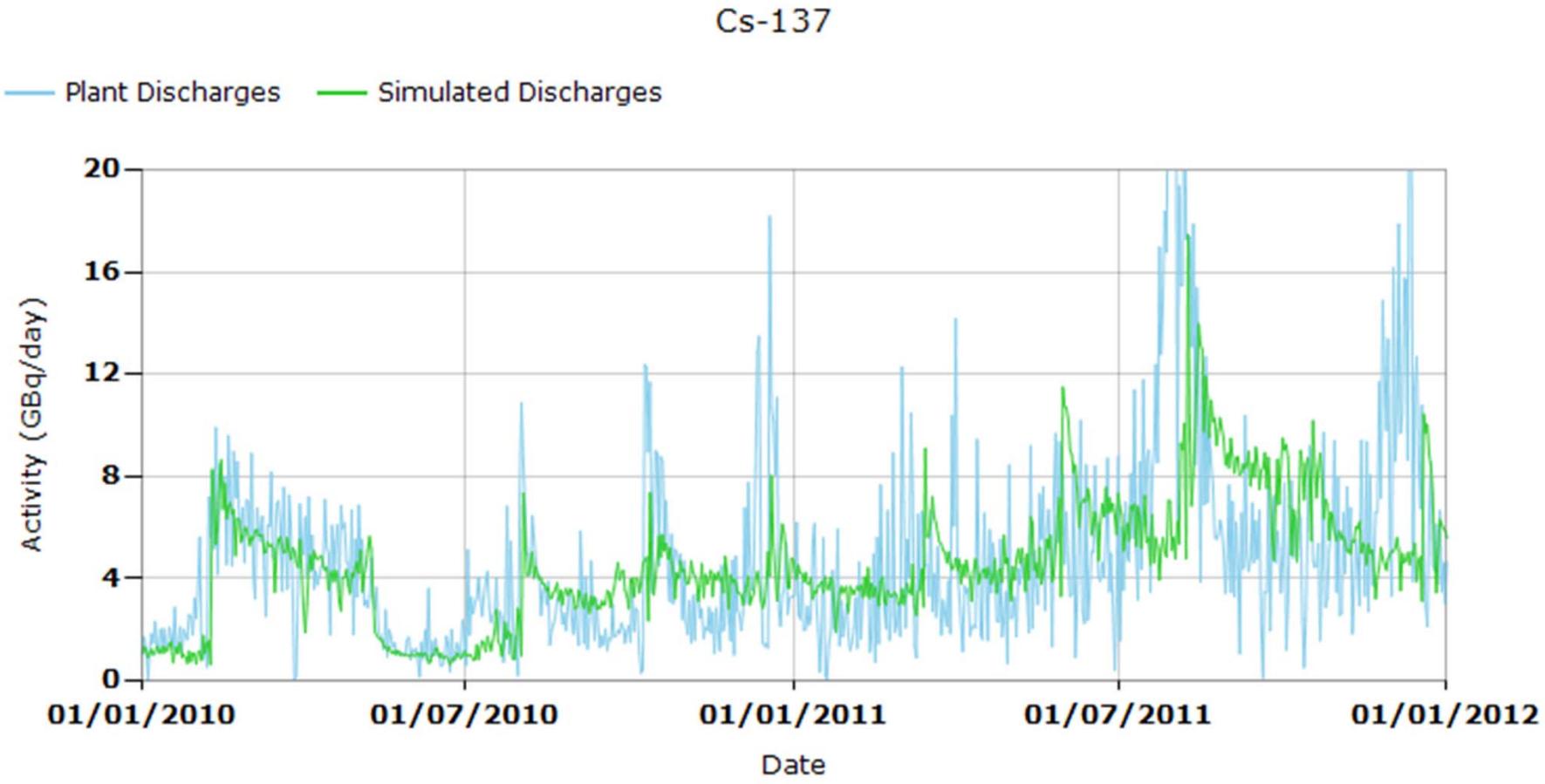
- Predict bed discharges



What can the model do?

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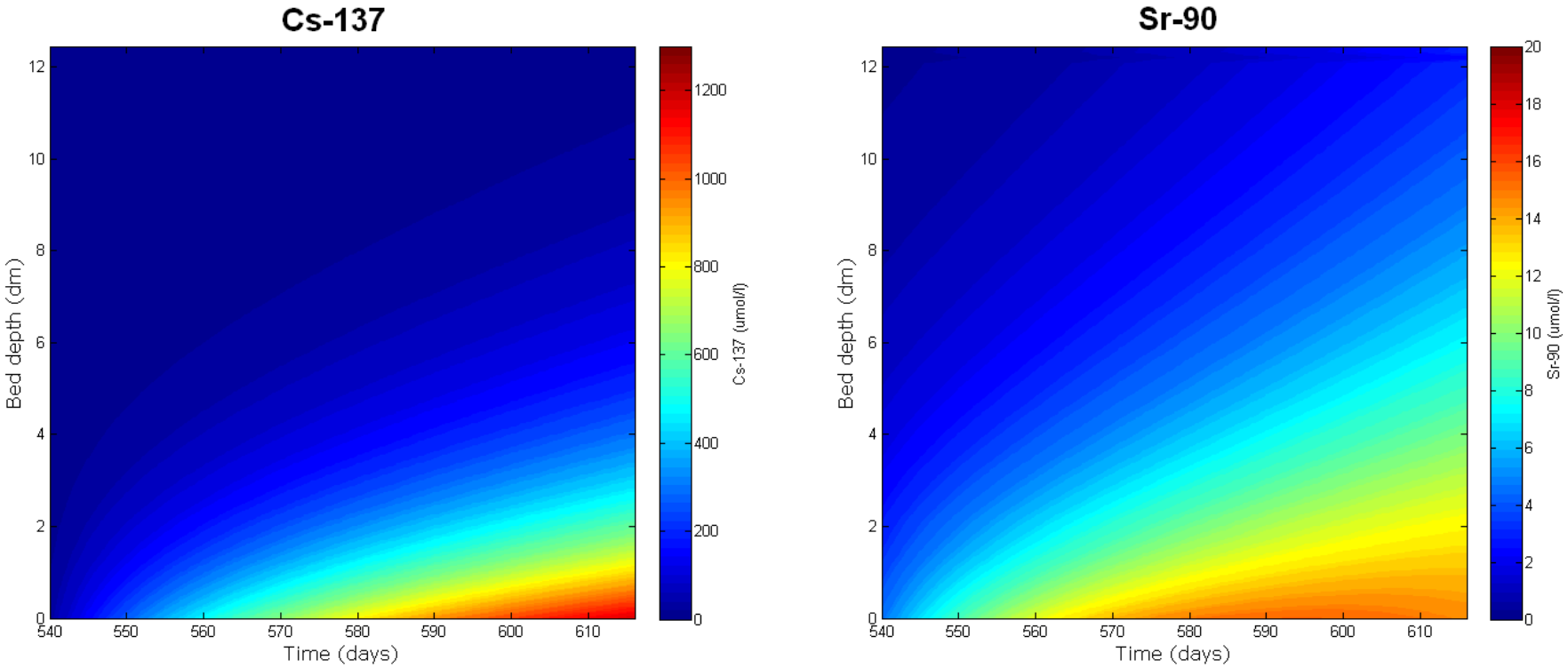
- Predict IX bed loading



Problem

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- Model detailed with long run times (1-10 hours)
- Significant number of scenarios required (and growing)
- Need to compare lots of scenarios
- Desktops not suitable

Use of Web interface

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- Solution
  - Automated web interface for gPROMS models
    - gO:RUN + FO / FPI interfaces

- Result
  - Runs use large computing cluster 24/7
  - Effective use of licences
  - Efficient use of time

NNL Modelling Web Interface

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NATIONAL NUCLEAR LABORATORY **Modelling Web**

Welcome, Jonathan Austin

Main Menu
- My Simulations
- View All Completed Sims
- View My Saved Charts
- Search Simulations
- Help
- About
- Update My Details
- logout

Admin
- User Accounts
- gPROMS Models
- gPROMS Versions
- Set Cluster Fingerprint
- Run Test Code

SIXEP Simulations
- New SIXEP Simulation
- SIXEP Plant Data
- Compare SIXEP Results

Model Development
- Model Development Home
- Create A New Model
- New Simulation Type

Validated Models
- View Validated Models
- New Simulation
- Compare Results

My Simulations

My Draft gPROMS Simulations

You have no draft simulations

My Running gPROMS Simulations

Simulation ID	Description	Status	Sim Type	Date Created	
3171	Test flow rate variations [4 of 4]	Submitting	SIXEP	09-Apr-2013	
3170	Test flow rate variations [3 of 4]	Submitting	SIXEP	09-Apr-2013	
3169	Test flow rate variations [2 of 4]	Submitting	SIXEP	09-Apr-2013	
3168	Test flow rate variations [1 of 4]	Submitting	SIXEP	09-Apr-2013	

My Completed gPROMS Simulations

Simulation ID	Description	Sim Type	Date Created	
3161	06872.301 - Final Heel Fitting, Plant, to Jan 2013 [New Purge feed] [1 of 1]	SIXEP	12-Mar-2013	
3160	06872.301 - Final Heel Fitting, Plant, to Jan 2013 [No SS] [1 of 1]	SIXEP	12-Mar-2013	
3148	06872.301 - Final Heel Fitting, Plant, Feb 2010 to Jan 2013, BSTs	SIXEP	11-Mar-2013	
3147	06872.301 - Final Heel Fitting, Plant, Feb 2010 to Jan 2013	SIXEP	11-Mar-2013	

NNL Modelling Web Interface

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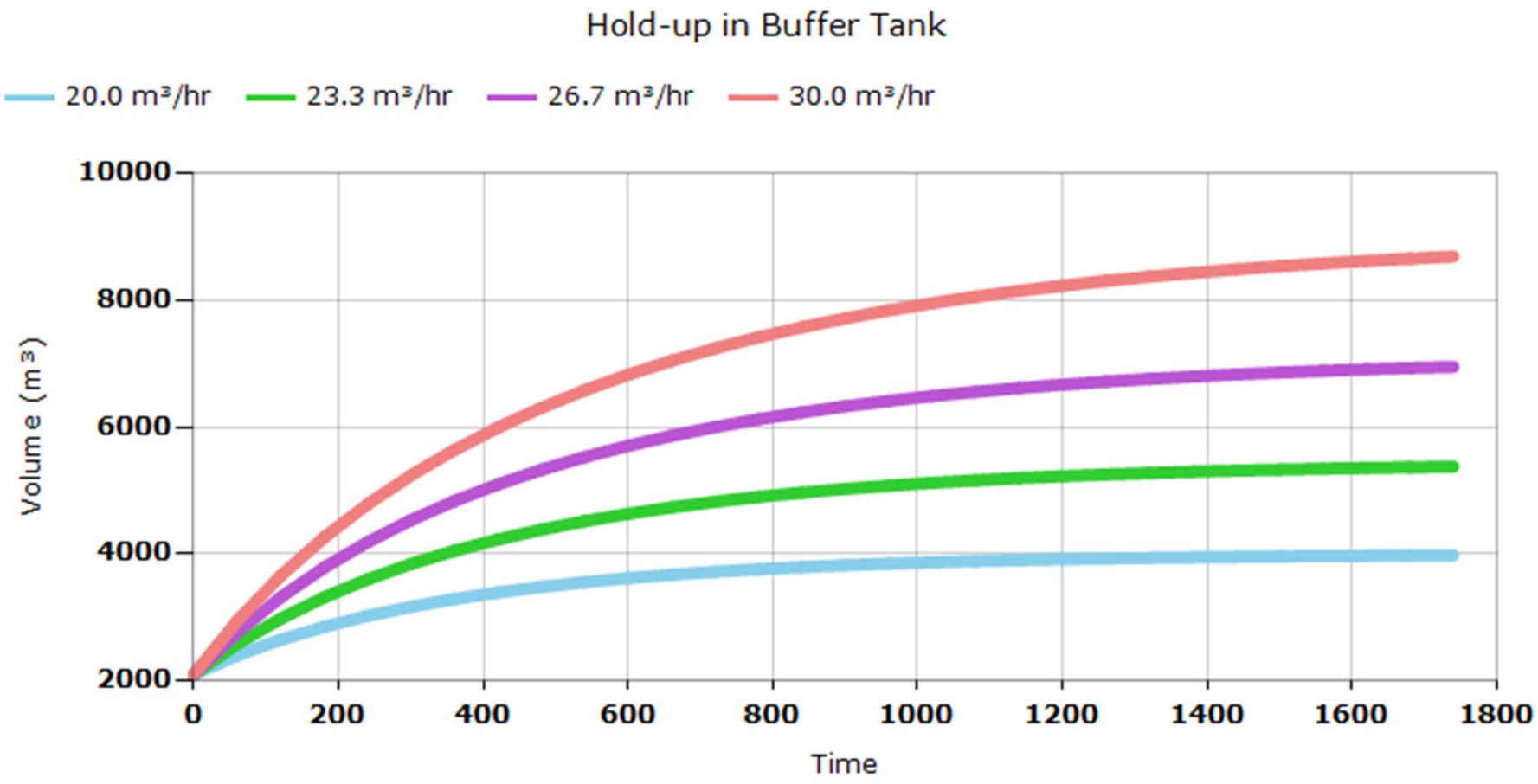

Model Development QA

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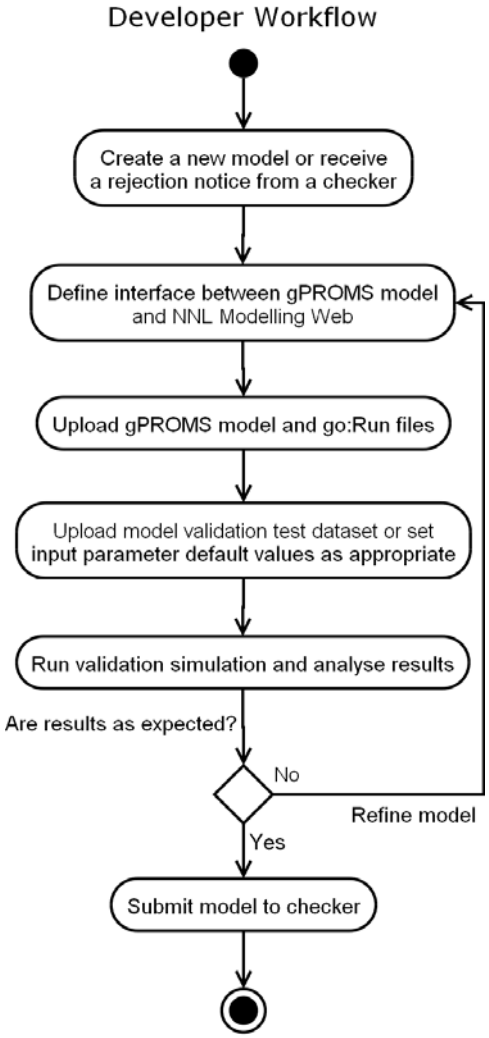

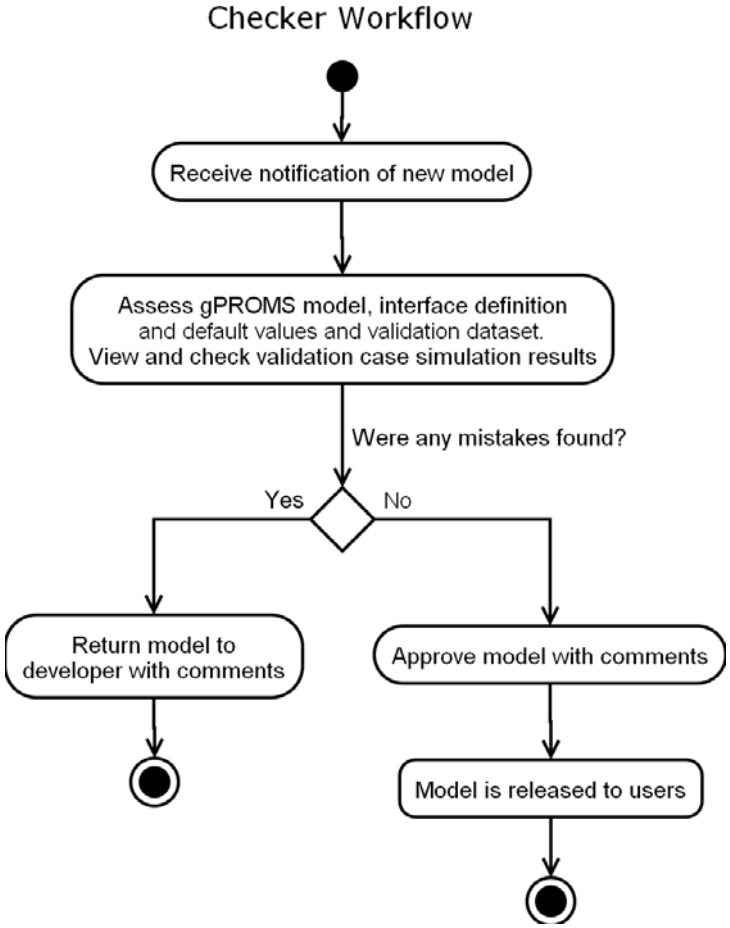

Running a Simulation

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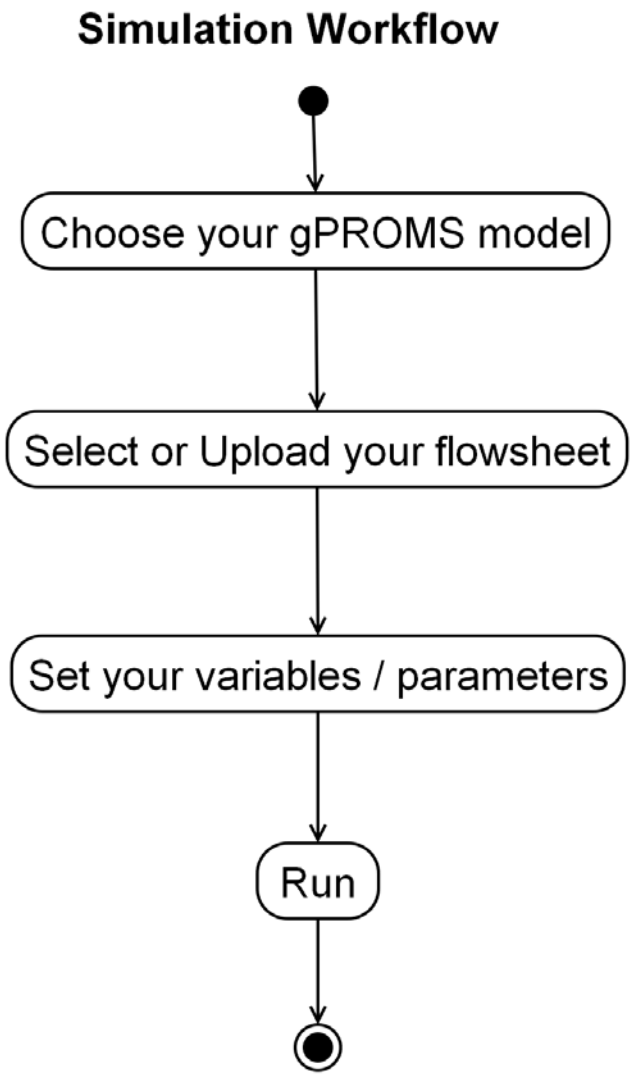

Example – Sensitivity Analysis

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- Feed sensitivity analysis:
  - Flow: 1000-3000 m^3/day – 5 steps
  - Cs-137: 1000-3000 Bq/ml – 5 steps
- 25 combinations
- ~2 hrs per sim
- ~50 hrs computation

Example – Sensitivity Analysis

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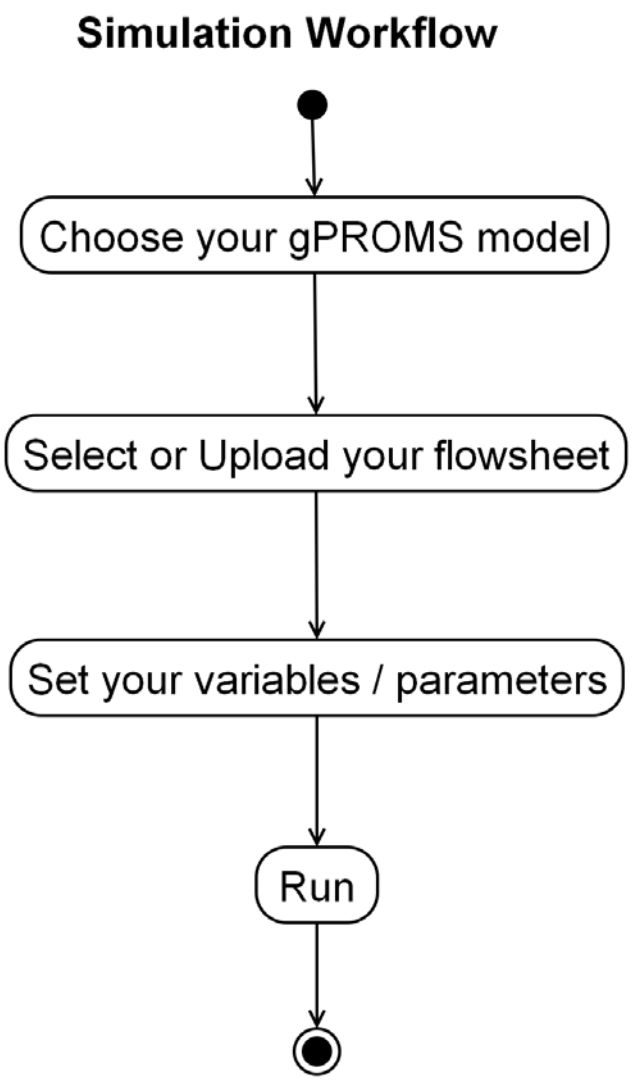

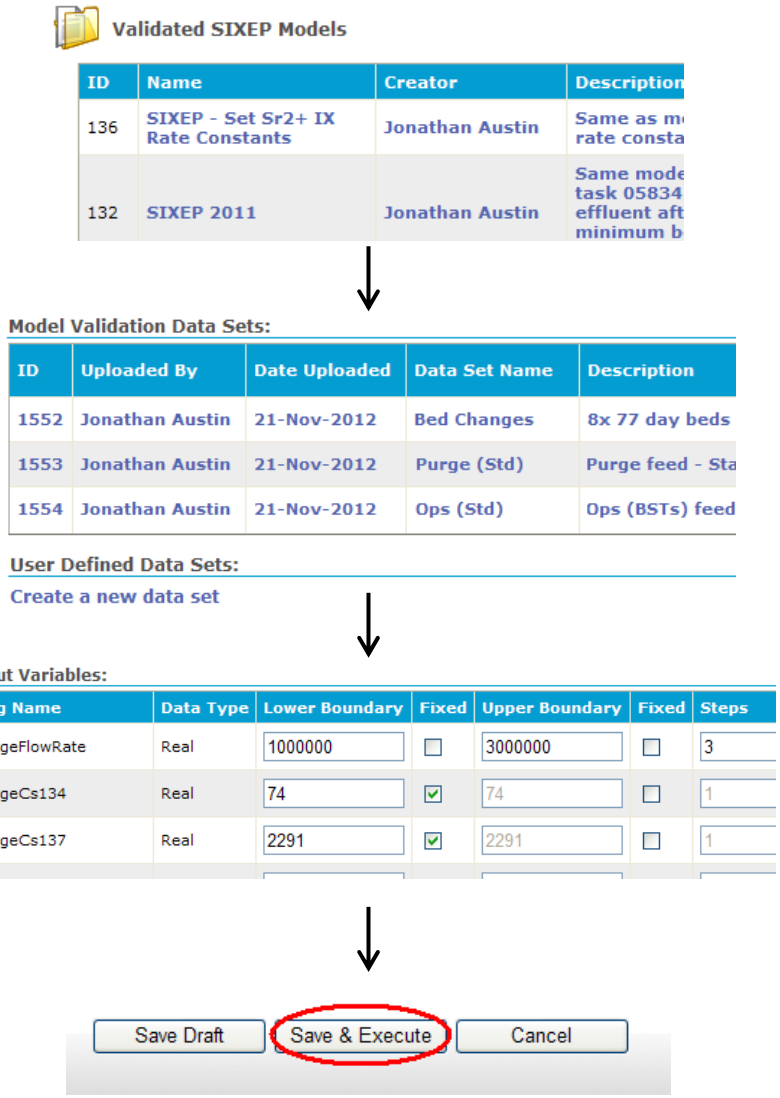

Compare Results

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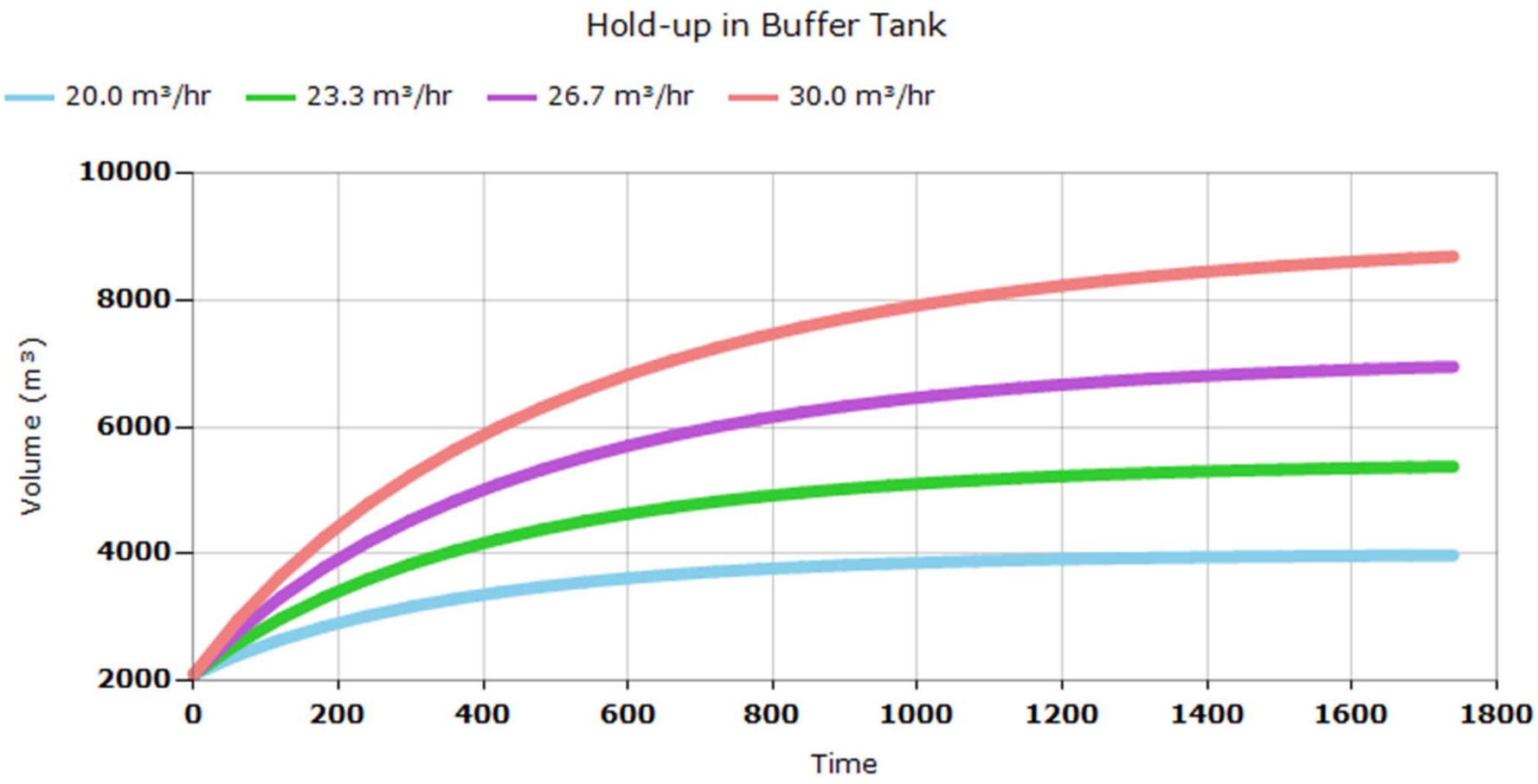

Project Successes - Model

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- Forecasts of plant performance
  - Predict plant discharges
  - Advise plant on how to manage IX bed changes
- Assess the impact of new feeds
- Demonstrate technical benefit of alternative IX material
- Underpin Plant Modification Proposals (PMPs)
- Underpin plant feed conditions for acceptance
- **The EA Endorsed Route To Accepting New Feeds**

Project Successes – Web Interface

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- Improve quality assurance
- Allow non-technical staff to run simulations
- Rolled out across a variety of NNL models
- Efficiency savings
- Model version control

Summary

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- Chemical and Process Modelling
  - A long established discipline in NNL which supports many plants and Processes
- SIXEP IX Model
  - A model that captures experimental and plant experience to give accurate predictions of plant performance
- Web Interface
  - An interface to gPROMS models that improves QA and efficiency

Questions?

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