WRMP24 Regional Plan

Simulation Model Scoping Report

WRSE

12 November 2019

Notice

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This document has 72 pages including the cover.

Document history

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Client signoff

Client	WRSE
Project	WRMP24 Regional Plan
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1. Introduction

Atkins was commissioned by Water Resources South East (WRSE) to undertake a scoping review of development pathways for a regional simulator, which is intended to perform a number of key roles within the overall WRSE assessment, as shown in Figure 1-1.

Figure 1-1 - WRSE assessment framework (Meyrick Gough, July 2019)

These roles have been expanded in Figure 1-2 and can be summarised as follows:

1. Determine baseline performance – simulate the current regional supply system and assess the impact, through the use of performance metrics, of relevant risks identified in the Resilience Framework.
2. Test options and groups of options – ahead of investment planning, appraise pre-existing options in terms of their capability to reduce baseline risk. This may allow some form of option preference to be applied for investment modelling.
3. Optimise operational rules and transfers – derive new transfer options which involve: (i) altering operational rules (possibly with implications for operational cost); (ii) varying the capacity of existing transfers; or (iii) new transfers.
4. Test and refine option portfolios – to support investment planning, appraise the benefits of different portfolios of options selected for different scenarios.

Following the scoping workshops and issue of the draft report the need was identified to generate 75-year supply / deployable output (DO) forecasts for use in the investment model. These would be based on, for example: current network configuration; optimised current network configuration; 1:200 drought resilience; 1:500 drought resilience; level of service alignment by 2040; level of service alignment by 2055; and climate change. It will also be necessary to determine the DO benefit of options within the context of these scenarios. This all represents a substantial volume of modelling with implications for programme length and, potentially, the development of other simulator functionality. Therefore, the approach to DO will be discussed and agreed as part of an early start task and an addendum to this report issued to reflect the outcomes of that early start task. Further information on the task is provided in Section 5.8.

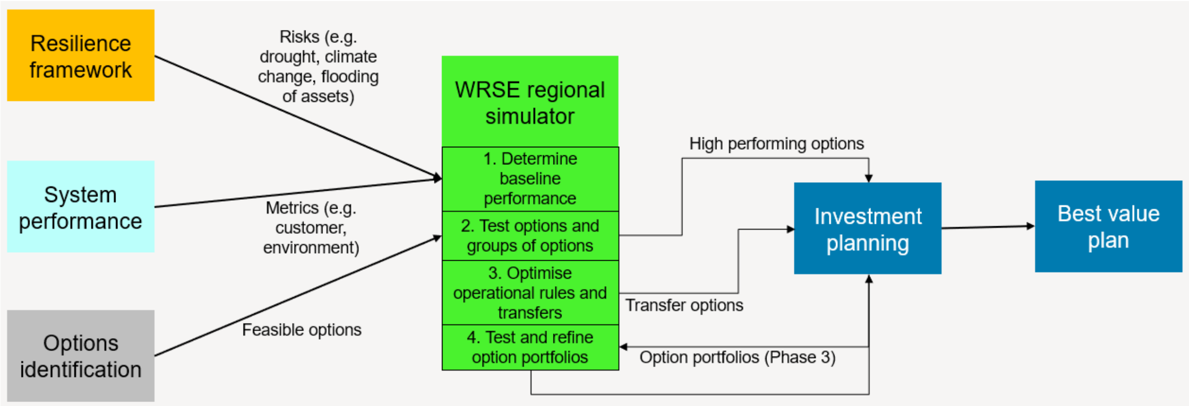


Figure 1-2 - Role of WRSE regional simulator

The development and running of the simulator will be undertaken in a phased approach. At the time of writing three phases have been defined:

- Phase 1 – Scoping, as outlined in this report
- Phase 2 – Development, testing, calibration, sign-off, primary and secondary runs (roles 1-3 above)
- Phase 3 – Assessment of option portfolios from investment planning (role 4 above) and initial steps to embed the simulator into full water company use (Section 4.5).

This scoping report summarises a detailed and wide-ranging review of approaches to developing a regional simulator for WRSE.

2. Overall scoping approach

In the broadest sense the regional simulator will consist of a network of models, tools, data and processes (see Figure 2-1), with a water resources simulator sitting centrally. The focus of this scoping exercise was to determine the most suitable development pathway for the simulator, considering all of the necessary connections and input data requirements.

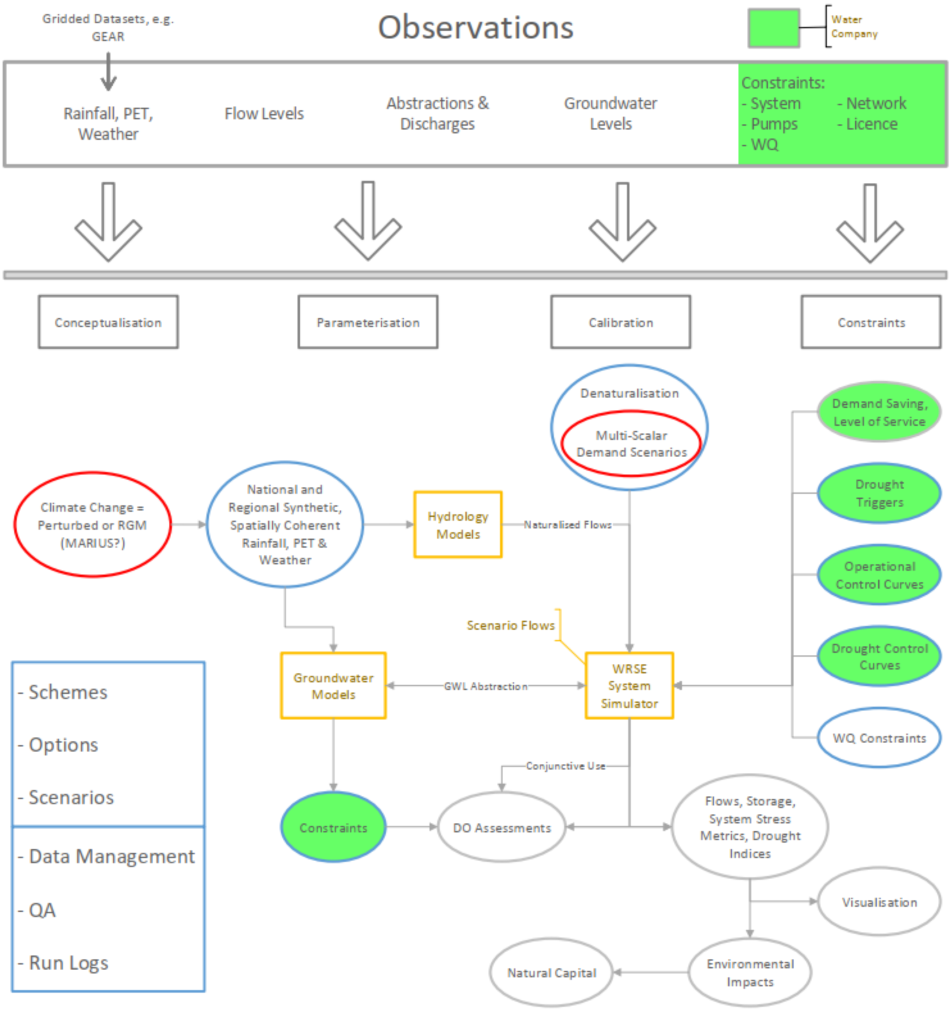


Figure 2-1 - Example diagram of a full regional simulation system (digitised from a sketch provided by Southern Water, August 2019)

The overall scoping framework is outlined in Figure 2-2 along with the project timeline. Engagement with stakeholders, primarily water company technical experts, was crucial to define the requirements, functionality and outputs that WRSE would need from a regional simulator. The first step of the review was to determine the requirements of the model from the following perspectives:

- Functionality – what features does the simulator required?
- Existing SE models – what model structure and level of detail is likely to be required?
- Data – what type and scale of input data are likely to be used?

Much of this information was collated during the interviews held with each water company's representatives. The available programme was also reviewed to impose a timeframe on simulator development, shown as Phase 2 in Figure 2-3. During the scoping exercise the start date was assumed to be 1st October 2019. However, at the time of writing this final scoping report (November 2019) a start date has not yet been confirmed, therefore the programme has been updated to show indicative month / week number from the (unspecified) start date throughout this document. The collated simulator requirements were prioritised in a workshop with the water company experts. The results of this exercise are documented in Section 3.3.

Different options for the regional simulator pathway were assessed in stages. A wide range of model platforms were considered against general criteria (Section 4.3) and those which were considered plausible were taken forward for detailed assessment, working through each of the specific prioritised requirements (Section 0). The different pathways were also discussed with water company technical experts during the interviews to capture their views.

The final recommendation for the simulator pathway was presented to water company representatives, at which point it was approved, and the feedback incorporated into this report. A model specification has been produced to assist with the tendering process for Phases 2 and 3 (Appendix A).

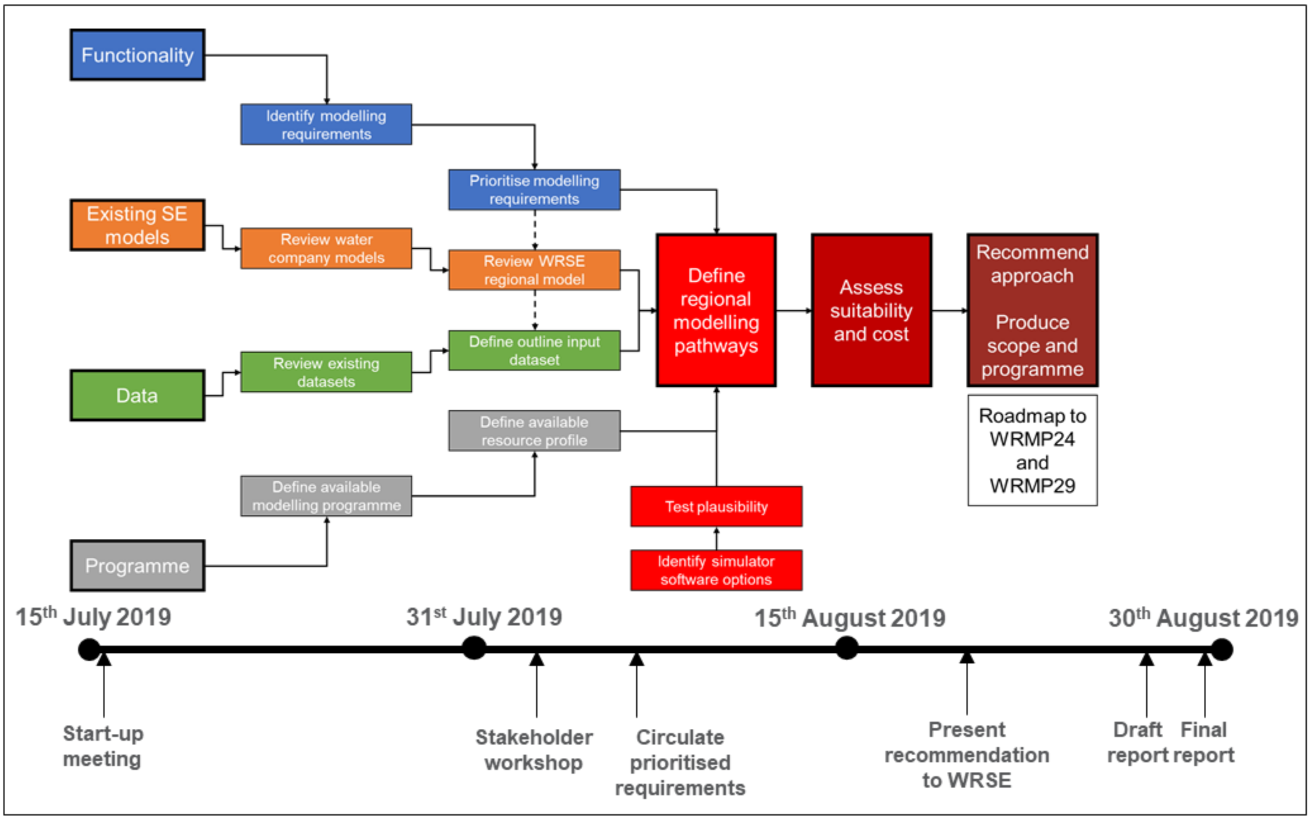


Figure 2-2 – Overall scoping framework and project timeline

Month 1	Month 2	Month 3	Month 4	Month 5	Month 6	Month 7	Month 8	Month 9	Month 10
Simulator development, calibration, testing and sign-off					Primary runs and analysis	Secondary runs and analysis		Sign-off and reporting	
Phase 2									

Figure 2-3 – Phase 2 timeline – approximate tasks by month from start date.

3. Simulator requirements

3.1. Approach

As outlined in Section 2 the requirements of the simulator were collated and prioritised to help select the most suitable simulator pathway. The list of requirements was created mainly by translation from the tender document (Appendix A), but also from information provided during the water company interviews and prioritisation workshop.

3.2. Collation of requirements

For each requirement a number of solutions were identified and the development implications of each set out. The applicability to individual companies was also explored during the water company interviews. This information was summarised in tables and used to inform the prioritisation workshop. These tables have been reproduced as Table 3-1.

Table 3-1 - Simulator requirements with potential solutions

F1 – Stochastic Input data

Understanding

The simulator should be able to process large amounts of synthetic (stochastic) input data.

Applicability to companies

Most companies are already using stochastic data.

Solutions

Full stochastics	Drought Libraries
Run the full stochastic sequences through the simulator. Timestep length could potentially be adjusted to allow longer sequences to be processed more quickly.	Filter stochastic sequences to identify a range of drought events and combine these into a shorter input sequence.
Implications • Simulator must be fast and/or have the ability to be easily parallelised to make running the full set of stochastics practical • Current WRSE simulator has already demonstrated this functionality.	**Implications** • Shorter runtimes • Less complete understanding of vulnerability. • Any system optimisations will be less robust.

F2 – Daily Timestep

Understanding

The simulator should run on a daily timestep. The previous simulator ran on a weekly timestep for computational reasons.

Applicability to companies

Generally applicable to all. Some specific requirements that increase the importance for example where MRFs are not using weekly averages (10-day MRF at Teddington).

Solutions

Daily timestep	Weekly
Use a daily timestep	Replicate approach of existing simulator
Implications • Computationally difficult – current simulator needs 24+ million timesteps to run all scenarios. • Able to replicate operational rules in company models more closely.	**Implications** • Some operational rules have to modified. • Fit between simulator and company models will be poorer. • Easier to run all scenarios.

F3a – System Optimisation

Understanding

Identify potential options to be used as input into the investment model by exploring connectivity and conjunctive use in the simulator.

Applicability to companies

Generally seen as critical except for Portsmouth Water whose bulk transfers have been shown to be resilient to a 1 in 200 event. Also, Affinity saw any optimisation of control rules as future work (DO of proposed transfers is most critical).

Solutions

Iterative manual optimisation	Manual optimisation
Optimise system by looking at performance against a range of constraints and objectives. Update rules/transfer iteratively using these performance metrics and align closely with investment modelling work.	Same as other solution but with less iteration and a limited consideration of new transfers (i.e. only consider those where there is an clear supply-demand gradient)
Implications • Feedback from investment modelling can inform work. • Process does not guarantee optimum solutions and cannot clearly quantify trade-off between objectives. • 6 months work.	**Implications** • Quicker (~1 month) • Solutions are even less optimal than an iterative process.

F3b – System Optimisation additional solution

Multi-Objective Evolutionary Algorithms (MOEAs)
MOEAs could be used to identify both portfolios of options and more optimum operating rules for the existing network. The functionality to link to MOEAs has already been built some modelling platforms (e.g. Aquator and Pywr).
Implications • Would produce sets of Pareto optimum solutions • Pareto fronts can show clears trade-offs between different objectives • Computationally expensive and would need significant setup time. This means that it is probably unrealistic for WRMP24 but the groundwork could be laid for WRMP29.

F4 – Adaptability of simulator to different conditions

Understanding

The simulator should be able to adapt to different conditions not previously simulated and produce sensible results that do not overstate the risk of failure.

Applicability to companies

Universal – Companies must have confidence that the simulator is producing realistic results, even under the more extreme scenarios.

Sustainability reductions a key theme here for some companies.

Solutions

Use optimised operational rules	Manual updates
Use the outputs from the system optimisation process (F2) to refine operational rules.	Update simulator in response to specific instances where it is producing unrealistic results due to the stochastic inputs.
Implications • Dependent on optimisation process being completed. • Takes a more holistic view of model performance. • Uncertainty over when simulator is 'complete' as approach implies that the simulator used in optimisation process is not.	**Implications** • Not coherent - each change could potentially have knock on effects that create further problems. • To some extent, this will be done as part of the model build process.

F5 – Temporary Outage Risks

Understanding

Ability to model temporary outage risks, for example due to flooding.

Applicability to companies

Important to most companies, e.g. significant concern over oil spills for Portsmouth Water. SESW (issues with flooding) thinks the focus should be on loss of DO. Some questions about whether this is the best tool to assess this type of risk. Thames Water models outage with a separate method.

Solutions

Monte Carlo Simulation	Outage Scenarios
Run simulator repeatedly with outage probability distributions of outage for each treatment works.	Assess outage risk outside of simulator and run specific scenarios in simulator to understand their impacts
Implications • Probabilistic outputs would provide a better understanding of risks • Requires thousands of runs which might not be technically feasible. • Could use company outage models data as inputs but potentially take some time to setup. • 1 month development time	**Implications** • No technical issues or specific changes needed to simulator. • Would provide less understanding of the combined outage risks. • Short setup times

F6 – Testing options / option portfolios

Understanding

Use the simulator to test the performance of the system / options / option portfolios using metrics against a range of scenarios and conditions.

Applicability to companies

A range of metrics for testing suggested in the interviews including: DO, different measures of reservoir storage / recession, environmental flows (e.g. time spent at HoF), supply deficits (frequency, duration), LoS restrictions, % of capacity utilised, focus on the flow left in the environment (SESW).

No call for metrics that would necessarily require specific model development (e.g. new functionality or additional nodes).

Solutions

Full stochastics	Drought library
Run each portfolio through full set of stochastics and scenarios and use metrics to assess performance. Replicates approach previously taken by WRSE.	Run a subset of stochastics an scenarios through the simulator
Implications • Computationally expensive – long runtimes. • More complete understanding of the robustness of portfolios. • Conditions where system is most susceptible to failure can be identified	**Implications** • Less computationally expensive • Less complete understanding of portfolio robustness/performance.

F7 – Deployable output

Understanding

Calculate DO at regional and sub model scales. Main focus expected to be at WRZ level for model development and testing.

Applicability to companies

Applicable to all. For companies where DO is expected to be the key metric this becomes more important. Need to take account of approach used by each company.

Solutions

Build DO analyser into Simulator	Custom scripts
Add the ability to carry out DO analysis to core simulator code.	Develop custom scripts to carry outputs specific DO runs externally to core simulator code.
Implications • Some models, such as Aquator, already include DO analysers, so no development time would be needed • Better usability. • Existing tools and outputs are familiar to users	**Implications** • Simple to implement in code so little development time. • Increased flexibility • Potentially easier to parallelise (useful when calculating DO for stochastics inputs) • Can be permanently added to simulator at a later date

F8a – Dynamic Groundwater representation

Understanding

Groundwater representation was identified as primary limitation of the existing WRSE simulator. This was because: i) groundwater dominated areas had to be oversimplified; ii) it was not possible to model the conjunctive use of surface and groundwater; and iii) it was not possible to use groundwater state as an indicator or metric.

Applicability to companies

A strong desire throughout the companies for better GW representation. Thames is SW dominated but the value of improved GW modelling is recognised. For some companies WRZs the constraints are linked to licence / asset capacity rather than hydrogeological conditions (can check this too as a screening step in development). Affinity could use recharge models to create input data with ADO, PDO varying by year applied in the simulator. A few companies already have lumped parameter GW models (e.g. Portsmouth and SESW)

Solutions

Incorporated the full regional GW models into simulator	Develop a lumped parameter model
Couple the simulator to regional groundwater models.	Use regional groundwater models to develop a statistical relationship between abstraction and groundwater availability.
Implications •Would be best possible representation of groundwater •Significant development time would be needed. • It is likely that runtimes would still be too slow to feasibly run long stochastic series through the model.	**Implications** • Run times should be fast enough to run stochastic data through the simulator • Development times would still be significant (6+ months) • Might not be possible to develop acceptable models for some aquifers • Would allow calculation of hydroecological metrics

F8b – Other Groundwater solutions

Use New EA groundwater model	Run GW/recharge models externally to create input timeseries	Use Drought index to reduce DO during severe droughts	DO profiles
Integrate with simulator or use outputs?	Run regional groundwater externally to provide timeseries inputs to the simulator	This is the approach taken in the existing WRSE simulator. Fixed DO profiles are modified when index indicates a severe drought.	Use fixed DO profiles for all groundwater sources
Implications • Need to investigate and understand the model. • Integration with simulator could be difficult and time-consuming.	**Implications** • Significant time needed to develop inputs. • Runtime of models may be too slow to feasibly create all the required inputs. • No dynamic GW response to model state.	**Implications** • Minimal impact on simulator runtime. • No dynamic GW response to model state. • Simple to implement, so little development time	**Implications** • Very easy to implement • Too simplistic for overall aims of the project.

F9 – Water Quality Representation

Understanding

It would be useful if the simulator was able to model the impact of quality on abstraction and the blending of water at different nodes.

Applicability to companies

Generally seen as a nice to have and one for the future. Slightly greater importance for Thames with simulation of the Severn – Thames Transfer.

Solutions

Add WQ functionality into simulator	Use input timeseries/profiles
The functionality could be built directly into simulator or the simulator could be coupled with an existing WQ model.	Calculate WQ timeseries and/or profiles externally (using existing models/ methodologies?) and use as input to simulator
Implications • Likely to have significant impact on simulator runtimes. • There are various approach to adding WQ functionality but all are likely to have 6+ months development time depending on the modelling platform.	**Implications** • Relatively simple to implement in the simulator. • Developing input timeseries profiles/timeseries could potentially be difficult. • Could also output blend ratios without any specific development

F10 – Operational drought management

Understanding

Extend the simulator to include operational drought management capable of demonstrating the likelihood of system failure over the coming months based on the simulation of current operational asset base, potential planned outage events and a range of likely climatic events, given the antecedent conditions to date. Help to plan regional operational interventions.

Applicability to companies

Variable response, Thames, SESW and SWS think this is possibly something for the future as the system becomes more connected. SEW think this is important as there is a gap in company plans in going from level 3 to level 4 restrictions. These droughts are likely to be felt at a regional level.

Solutions

Use climate forecasts	Use stochastic data
Use climate forecast to generate/ modify simulator inputs to create a range of future predictions.	Extract plausible timeseries from stochastic data and use to forecast probability of failure. Use the model to output suggested operation actions
Implications • Significant development time (~1 year) • For usability, a custom user interface for the tool might be required.	**Implications** • Relatively simple to implement method • ~3 months development time.

F11 – Natural Capital

Understanding	Solutions	
Use simulator to make predictions of natural capital changes	**Incorporate directly into the simulator**	**Use simulator outputs to calculate natural capital**
	Modify the simulator so that it calculates natural capital during each timestep	Create a postprocessing tool to calculate natural capital from simulator outputs
Applicability to companies	**Implications**	**Implications**
Applicable to all companies and considered beneficial, however not seen as an immediate priority (seen as outside of the simulator scope by Affinity). Highlighted that it should be investigated with simulator outputs rather than within the simulation.	• Significant development time (~ 6 months) • Would likely add significant complexity to the simulator and impact runtimes	• Simpler to implement though it would also likely require changes to simulator structure so that required data could be captured • Would not be possible to use natural capital directly as an objective/constraint in any optimisations.

F12 – Multisector representation

Understanding	Solutions	
Include demands/requirements of other sectors, such as agriculture and energy directly in the simulator It is crucial to understand the objectives here. To account for other impacts of other sectors in water supply planning? To provide information to other sectors to assist their planning?	**Incorporate fully into simulator.**	**Limited representation**
	Try to incorporate other sectors into simulator in as much detail as possible	Limit representation to major impacts or aggregated multiple impacts into single nodes.
Applicability to companies	**Implications**	**Implications**
Mixture of views from nice to have to fairly important (e.g. SWS). Thames stressed that RWE Didcot was necessary to include in the simulator.	• Development time likely to be fairly limited although could lead to expansion of model structure with some penalties for run-time. • Potentially useful for multicriteria optimisations.	• Insufficient detail for many uses • Little impact on development time and runtime.

F13 –Visualisation

Understanding	Solutions	
Make use of innovative visualisation techniques to communicate simulator outputs (and workings) to technical and non-technical stakeholders.	**Standalone application/dashboard**	**Create visualisation for specific outputs and make use of inbuilt simulator visualisation tools**
	Create a standalone application that would allow users to explore simulator outputs in depth (and potentially wider WRSE outputs). This would use web-technologies to add interactively and GIS functionality. Could be distributed to stakeholders either as a desktop application and/or website	Create separate tools/apps to visualise specific outputs (e.g. portfolios) and make use of visualisation tools that some of the modelling platforms have built in.
Applicability to companies	**Implications**	**Implications**
The ability to engage with stakeholders from a variety of technical and non-technical backgrounds is paramount. Clear and effective visualisation is seen as an excellent vehicle to achieving this. All companies agree. The functionality to map outputs from region to resource zone to catchment would be very powerful.	• ~3 months development time	• No single tool and consistent approach for viewing results • Potentially inconsistent styles • Less development time

F14 – Usability

Understanding

It is important that the simulation model can be used and maintained by the WRSE / member water companies.

All solutions will require good documentation and training material.

Applicability to companies

Mixture of responses with some companies wanting to use the model fairly comprehensively (SWS), some wanting to be able to drill down into certain model operations (e.g. Affinity assessing transfers), others some wanting to run scenarios (Portsmouth) and all wanting to be able to see how results / decisions have been processed by the model (audit trail vs "black box").

Solutions

Graphical User Interface (GUI)	Command Line Interface (CLI) and/or scripts/notebooks
Simulator can be setup and run from a graphical user interface. Could be Desktop and/or web-based. Solutions already exists for most modelling platforms and are familiar to many users	Similar approach to existing WRSE simulator. The simulator could be run both via a CLI and via scripts/python notebooks.
Implications • Development time depends on modelling platform • License costs (platform dependent) • Less flexibility	**Implications** • Quicker to develop and more flexible. • Potentially easier to parallelise and run on the cloud. • Less accessible. • Depending on modelling platform, likely to be developed prior to GUI in some cases.

F15 – QA

Understanding

Good QA is essential for providing confidence in the simulator build and outputs. This is particularly important for development pathway 2, where the simulator is unlikely to be 'signed-off' unless robust and comprehensive QA can be demonstrated.

Applicability to companies

QA seen as very important to all companies. A clear view was expressed that a strong QA process yields long-term benefits for short-term effort.

Solutions

Distributed version control system	Manual QA
• Use a version control system, such as Git, to track code changes. • Host code on version control platform such as GitHub or Gitlab to allow collaboration and code review. •Write unit test for all code • Use continuous integration and issue tracking	Use logs to track changes to simulator and data
Implications • Less applicable to some modelling platforms. • Security – where will the code be hosted?	**Implications** • Easier to setup • Familiar to more people.

F16 – Data Management

Understanding

Large amounts of data will be generated both as inputs to and outputs from the simulator. It is a priority that this data is properly managed and stored in a way that minimises chances of errors.

Solutions

Custom Database	Traditional folder structure
Create a standalone database containing all input and output data. This could potentially be linked / extended to other WRSE work packages.	Store data in a traditional folder structure. Individual inputs/outputs can be stored in most suitable formats (e.g. NetCDF, h5, csv, etc..) for their particular characteristics.
Implications • The varied nature of the inputs and outputs (in terms of size, shape, format etc…) make it difficult to develop a single solution. • Some modelling platforms have a version of this but potentially have limits of the amount of data.	**Implications** • Familiar to users • No development time • Can be cloud based to make sharing easier. • Less consistency

3.3. Prioritisation of requirements

The model requirements were prioritised in a stakeholder workshop held in August 2019. Table 3-2 lists the functionalities, with the priority set at high, moderate or low. In general, these may be classified as:

- High priority: means that the functionality must be included within the Phase 2 simulator build ready for testing in 2020;
- Moderate: means that it is important but that there is some flexibility around the timing and/or level of detail;
- Low: means that it is a functionality that is either not needed or that can be added at some unspecified point in the future.

The workshop also provided the opportunity to discuss the approach to many of the development tasks, for example the simulation of groundwater. This information is summarised in the table and was fed through into the development of the programme (Section 5.3) and model specification (Appendix A).

Table 3-2 - Prioritised simulator requirements

Simulator requirement	Priority	Description/notes
F1. Stochastics	High	Simulator must be quick enough to run with the full stochastic data inputs (20,000 years +) in a practical amount of time. Drought libraries, developed from analysis of the full stochastic run outputs, can then be used for more detailed analysis, such as option identification and testing. It is anticipated that these data would be delivered under a separate workstream.
F2. Timesteps	Moderate / high	It is a high priority that the simulator can run on a daily time step. It is a moderate priority to also include weekly timestep functionality. Ideally the simulator would be able to switch between the two. Weekly timesteps would speed up the running of the full stochastic dataset while the daily timesteps are important for the detailed investigation of specific events/ drought libraries and matching the operating rules of the company models.
F3. Identification and optimisation of transfer options	High	This must be included and meet the deadline to feed into investment modelling. Process taken to test options should be clear, iterative and easily understandable, not a ‘black box’. Any changes made to operating rules need to be presented as their own options. The initial focus should be on major strategic transfer options. Method used will be manual and iterative with some feedback from the investment modelling, but the aim is to use Multi Objective Evolutionary Algorithms (MOEAs) in the future.
F4. Adaptability of simulator to different conditions	High	It is important that the simulator gives sensible results when simulating new conditions found in the stochastic data. This will require iterative testing throughout the development of the simulator. The simulator will be validated against historic DO calculated from company models, but where possible, companies will also run the stochastic data through their models (see F7 also) to allow comparison of system response to different conditions.
F5. Outage	Low	Not an initial priority but something that would be useful for the next round of plans. Simulator should help companies understand the impacts and consequences of big outage events (e.g. regional power failures). Simulator will be used for testing system resilience and identifying potential resilience options.
F6. Option/Portfolio testing	High	Assess performance of options and portfolios.

		Metrics to assess the options to be identified and agreed. This could include consideration of metrics to test performance in other sectors (e.g. agricultural). The impact that some metrics may have in terms of required changes to the model structure and therefore runtimes will need to be considered.
F7. DO	High	The simulator must be able to calculate DO, as validation against company model DOs will be key to sign-off on the simulator. The development of drought vulnerability surfaces will also be required. It would be useful if this was an inbuilt feature (i.e. not custom code/scripts), but flexibility would be beneficial so that company-specific DO assessment methodologies can be replicated as easily as possible. An action from the workshop was that companies will need to run the full stochastic datasets through their models so that stochastic DOs calculated by the simulator can be validated (or drought libraries where running the full dataset through the company's model is infeasible / impractical, for example for Thames Water's WARMS2 model). Following the scoping workshops and issue of the draft report, a further requirements was identified: to generate 75-year supply / deployable output (DO) forecasts for use in the investment model. These would be based on, for example: current network configuration; optimised current network configuration; 1:200 drought resilience; 1:500 drought resilience; level of service alignment by 2040; level of service alignment by 2055; and climate change scenarios. It will also be necessary to determine the DO benefit of options within the context of these scenarios. This represents a substantial volume of modelling with implications for programme length and, potentially, the development of other simulator functionality. Therefore, the approach to DO will be discussed and agreed as part of an early start task (to be agreed with WRSE), and an addendum to this report which would be issued to reflect the outcomes. Further information on the task is provided in Section 5.8.
F8. Dynamic groundwater	High	Dynamic representation of groundwater (and surface water interaction) is an important functionality of the simulator. Use of company groundwater models within the simulator was ruled out due to complexity and runtime issues. Companies will need to carry out a vulnerability/risk assessment of their Groundwater blocks early in the simulator build phase to prioritise development and inform representation of those prioritised groundwater units in the simulator. Those blocks that have dynamic surface water–groundwater interactions will require the development of lumped parameter models. For other groundwater blocks, either an input timeseries or a DO profile (with drought impacts) could be used, depending on the characteristics of that block and the existing models of it. River gravel abstraction could potentially be modelled as run-of-river surface water abstractions. It will be important to have a clear and auditable way of mapping each groundwater block to the different possible representations in the simulator.

		Confidence in simulated environmental outcomes is important and adequate time, data and understanding are required in order to achieve this. Assumption is that a significant proportion of the total groundwater DO of the WRSE region will need to be represented dynamically in the simulator (i.e. there will need to be good justification for not representing a block dynamically). The importance of including dynamic groundwater varies across WRSE companies. In the Thames catchment, improving the representation of hydrology was seen as a higher priority. Developing a groundwater risk assessment framework was identified as an early start task; more information is provided in Section 5.7.
F9. Water Quality	High/ Moderate	Should be treated as two individual issues: raw water quality and treated water quality. It is a high priority that water quality is included in the initial simulator build as a series of constraints on abstraction / works treatment capacity. Water quality / algal bloom impacts could be included as external rules / input timeseries of risk that constrains output when the risk is above a threshold. It should also be possible to extract blend ratios from the simulator outputs. In the future (i.e. beyond WRMP24) the simulator should be able to model water quality directly using an empirical approach, for example as implemented in the SAGIS / SIMCAT water quality model. Some water quality constraints will still likely be too complex to represent directly in the regional simulator, such as algal blooms. These could be investigated separately in more sophisticated water quality models such as MIKE Ecolab and the outputs translated into some form of constraint to be applied in the regional simulator.
F10. Operation drought Management	Low	Extend the simulator to include operational drought management capable of demonstrating the likelihood of system failure over the coming months based on the simulation of current operational asset base, potential planned outage events and a range of likely climatic events, given the antecedent conditions to date. Potential to incorporate seasonal weather forecasts into the system, though this would likely require significant development time. Not a high priority for the next plan but will be needed eventually.
F11. Natural Capital	Low	Simulator will be used to inform Natural Capital assessment drawing on model outputs. Implications for model structure (e.g. additional nodes). Natural capital will feature more heavily in the investment modelling but there will be some feedback into the simulator, potentially using an increasing cost function.
F12. Multisector representation	Moderate	Workshop identified two separate aspects of multisector representation: 1) Impacts that need to be included as part of the denaturalisation process and 2) Failure of private sources during severe droughts that may place extra demand on the water companies (this would require a review of the performance of private sources during droughts). It is also important to consider multisector benefits when testing and identifying options.

F13. Visualisation	High	Priority to support validation and QA, and exploration / visualisation of data. Discussion of potential for development of a web-based application that could also be used for visualisation of outputs from other works streams (e.g. investment modelling). Needs to be interactive and allow users to explore simulator outputs in depth while also being able to communicate complex outputs to non-technical users. Should be developed alongside the simulator so that it can be used as a testing tool. Link to GIS for visualisation. Must have the ability to download raw data, link to GUI, GIS, and enabled the auto-population of WRMP tables.
F14. Usability	High	Important that training is provided to companies on model use so that they can run and tweak the model themselves. Preference for a web-based modelling platform that includes the ability to hide sensitive data and limits the changes users can make to specific geographic sections of the simulator. The platform should maintain a locked-down master version of the simulator. Secure access and data confidentiality: action for companies to review what datasets are sensitive and should be hidden. Atkins to explore options to secure data and model integrity.
F15. QA	High	Need a comprehensive and ongoing QA process as without good QA, the companies will not be able to 'sign-off' on the simulator. Bad QA also heightens the risk of external challenges. Given the tight schedule, as much QA as possible should be automated. A distributed version control system should be used to track model development and enhance collaboration Unit tests should be considered for any custom code written as part of the simulator development to provide confidence that it works correctly. Continuous integration could be used to ensure a smoother development process.
F15. Data Management	High	There should be a universal solution for data management that supports the simulator, any visualisation tools, and the other workstreams (e.g. investment modelling, options identification).
F16. Costs	Moderate	The workshop highlighted that it was important that costs are integrated in the model. There is some uncertainty about how the model will use these costs. They could be used for the allocation of resource on a per timestep basis and/or an objective to use in manual/automatic optimisation and identification of options. It was noted that the use of costs for allocation of water resources, such as in Aquator, does not always work that well. There is a risk that the cost estimates from different companies will not be comparable and it will therefore be difficult to use them directly in the simulator.
F17. Dynamic demand	Low[1]	The use of dynamic demand forecasts in the model will be explored.

[1] Subsequent to the workshop Anna Wallen suggested this priority should be increased to moderate, however this has not been discussed and agreed by WRSE.

F18. Bidirectional links	Moderate	The simulator should have the ability to represent bidirectional links. In most modelling platforms this can be represented using two transfers, though this method can give strange results (i.e. sending water in both directions). The alternative would be to build the functionality in at the solver level where the direction would be a binary decision variable, however this is likely to make the model much slower.
F19. Inter-regional transfers	High	Simulator should be able to model inter-regional transfers as fixed or timeseries inputs into the WRSE system.

3.4. Regional model structure

The current WRSE Pywr model structure is shown in Figure 3-1. The model is simplified relative to many of the individual water company models, particularly in the case of Thames Water and Southern Water. Many of the supply nodes are “non-simulated” (blue circles), meaning that inputs are represented by fixed profiles or timeseries of deployable output (DO). A number of reservoirs are “simulated” (red circles), i.e. the inflows, storage levels and abstraction rates are all computed within the run.

Due to the difficulties in simulating groundwater storage in a water resources model, only 42% of the DO in the model is simulated. A higher proportion of simulated DO would improve understanding of risk and resilience. Another key area for development, as highlighted by this schematic, is to provide better visualisation of the model and model outputs.

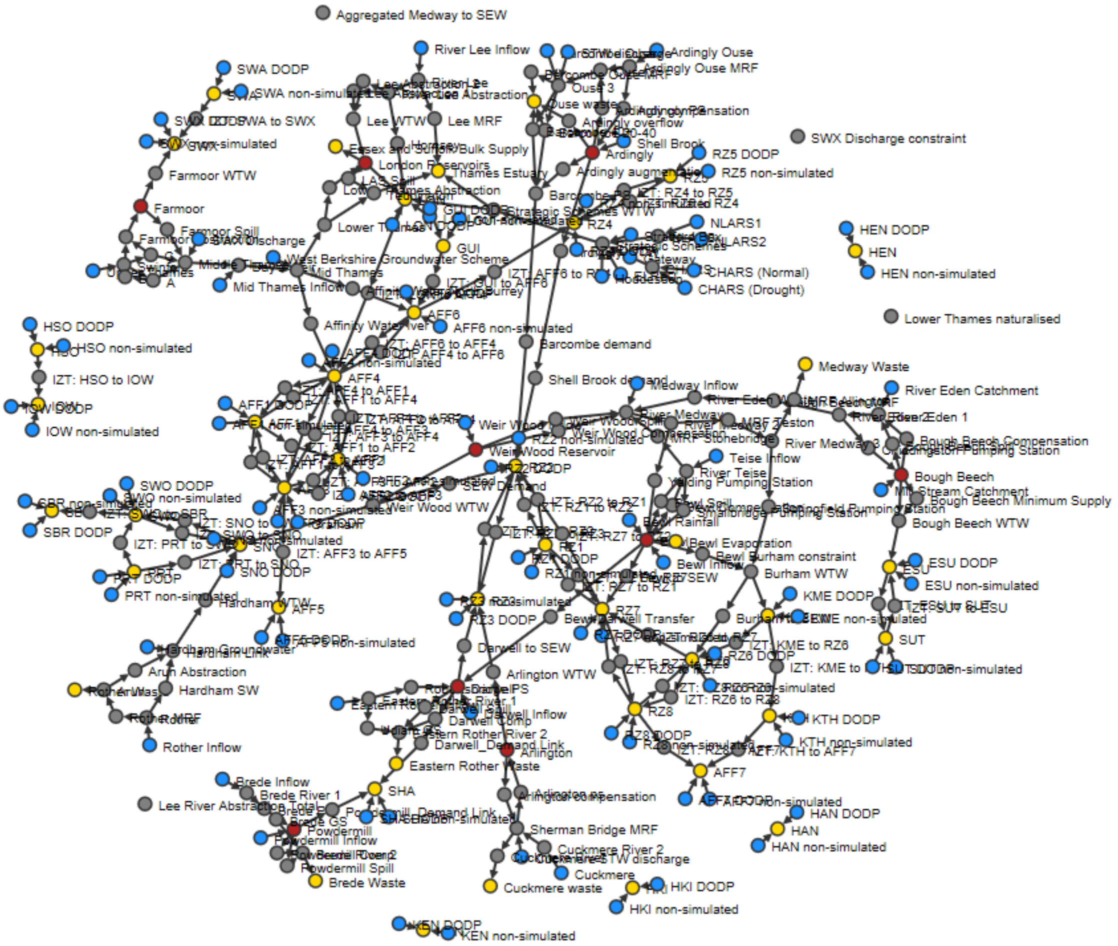


Figure 3-1 - Schematic showing existing WRSE Pywr model structure

As part of the scoping exercise a new draft model schematic was created with input from water company technical experts (Figure 3-2). It is important to stress that this will need to be further developed and refined within Phase 2; its purpose here is to:

1. Inform the simulator pathway selection process – model complexity is a key constraint on model development and run time.
2. Inform the Phases 2 and 3 tendering process by allowing bidders to understand the likely model structure and level of detail and complexity involved.

It has not been possible to finalise this in Phase 1, in part due to timescales, but also due to a need to perform model testing to ascertain exactly what detail is required. It was clear during the interviews that more detail will be required in the Thames Water and Southern Water areas relative to the previous modelling. However, as this will have a run time penalty it should only relate to areas that significantly influence model performance. The final level of detail is likely to sit somewhere between the simple structure shown within the map and the complex structure shown in the inset boxes (company Aquator schematics). The objective of testing in Phase 2 will be to determine which detail is required to achieve satisfactory performance, working closely with the companies to agree these details.

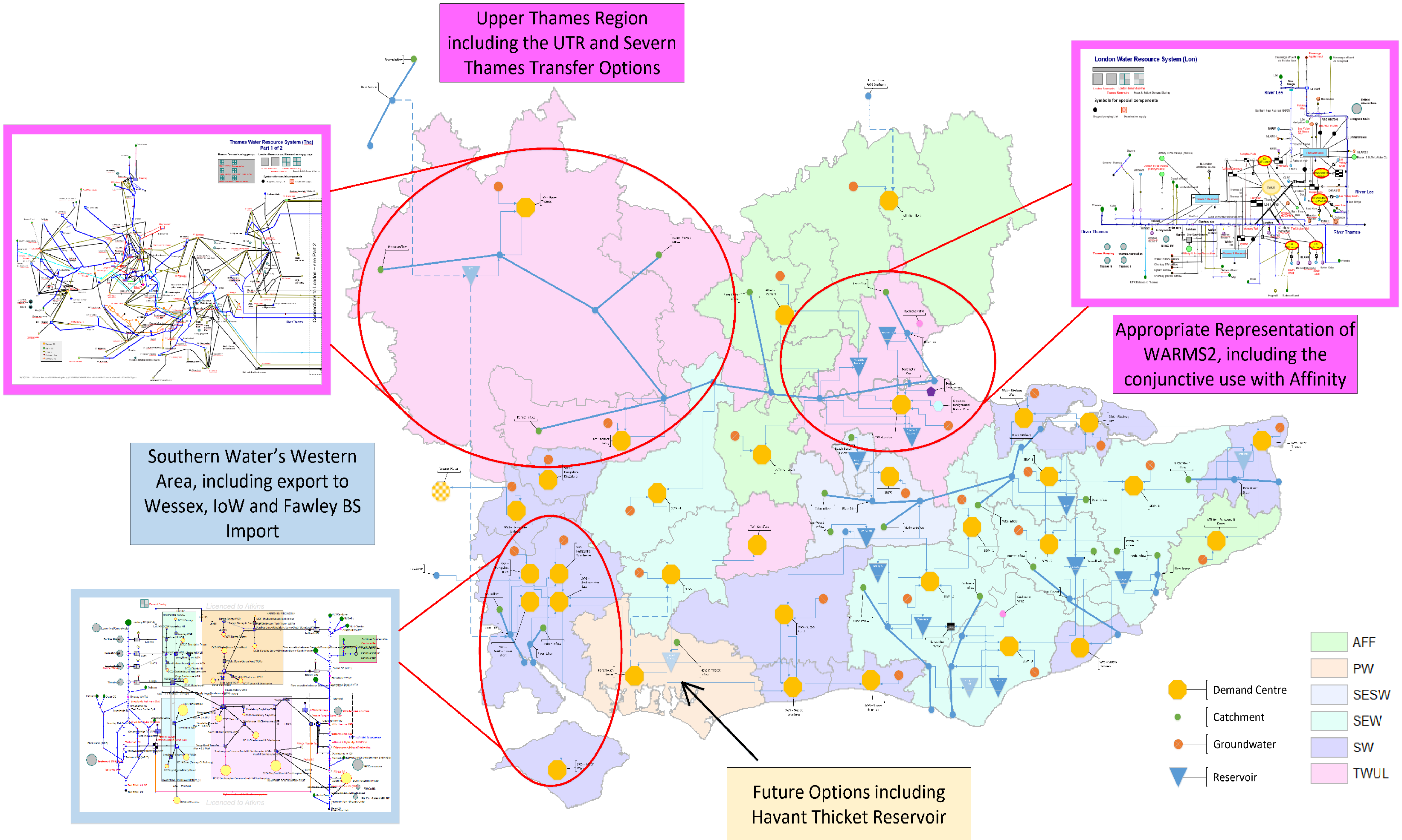


Figure 3-2 – Draft WRSE regional simulator model structure

4. Assessment of simulator pathways

4.1. Approach

The simulator pathway can be considered as two elements:

1. The primary pathway, i.e. the modelling framework / architecture
2. The modelling platform / software package to be used

For example, one primary pathway is a full regional simulation model but this could then be developed using a range of different software packages such as Aquator or Miser.

As noted in Section 2, the assessment of simulator pathways was undertaken in a series of steps:

1. A review of primary pathways
2. A broad assessment of modelling platforms according to a set of criteria selected to reflect the general WRSE simulator requirements
3. A detail assessment of plausible platforms identified in Step 2 against the specific prioritised functionality requirements, as set out in Section 3.
4. A final recommendation of simulator pathway

The outcomes at each stage are summarised in the following sections.

4.2. Primary pathway and the sign-off process

The tender document proposed three pathways for consideration as shown in Table 4-1.

Table 4-1 - Primary pathways considered

Option number	Pathway	Details
1	Universal platform	Some form of tool developed in Python, Excel, etc. to run all of the company models automatically, passing information between the models at each time step.
2	Fully signed-off regional simulator	A regional simulator which meets all of the agreed performance requirements. It could be developed in a range of platforms subject to assessment of suitability.
3	Regional reduced functionality simulator combined with company models	A regional simulator which does not meet all of the agreed performance requirements but still adds value when used alongside water company models as a reduced functionality simulator, for example to: • Help develop regional options for testing • Act as a tool for screening scenarios of future uncertainties such as drought and climate change • Provide regional boundary conditions (e.g. transfer or river flow) for the company models.

Option 1, the universal platform, was excluded at the outset due to the following technical reasons:

- Much of the required simulator functionality would be infeasible due to runtime
- Passing information between different models and platforms (e.g. Aquator and Kestrel) would be technically challenging, especially in terms of communicating allocation procedure variables such as “resource state”.

All companies agreed the aim should be to develop a regional simulator that is fully “signed-off” (Option 2). The preferred testing metrics were discussed during the interviews. These varied from company to company and included comparisons of deployable output, reservoir storage, river flow and groundwater abstraction. Early in Phase 2 the sign-off process will need to be further discussed and agreed with companies, and then a clear plan communicated (or this could be done as an early start task prior to commencement of Phase 2).

Other suggestions put forward by companies for sign-off included having a staged and iterative process. For example, a system schematic could be developed that would require sign-off as a concept, but then need revision after evaluation of calibration run outputs that showed where further modification of the system detail might be required. This process should also include consideration of any opportunities to rationalise the model structure. From a development perspective the principle objective should always be to produce a model which has the minimum possible level of complexity required to achieve the desired level of performance. Any superfluous complexity will increase development and run time which could potentially constrain simulator functionality.

Sign-off would require the delivery of a calibrated model achieving defined acceptance criteria. The process would need to take account of ongoing company model development, possibly with some phased migration. However, due to the development timescales available in Phase 2 this would need to be relatively constrained, with firm “lock-down” points.

Option 3 provides a “Plan B” in the event that the model cannot be fully signed-off, but still delivers value as a system “reduced functionality simulator” to work alongside the water company models. It is common to use this type of model alongside more detailed and accurate models, working together in a modelling suite. A decision will be taken following a progress review as shown in Figure 4-1 and the development roadmap (Section 5.2). However, to reiterate, the primary objective should be to develop a fully signed-off regional simulator.

Thames Water’s experience of using IRAS alongside WARMS2 highlighted the risks of using a “Plan B”-type reduced functionality simulator. As such, Option 3 will also need a sign-off step, the details of which should be discussed and agreed early in Phase 2. The role and purpose of the reduced functionality simulator should be clearly explained to stakeholders and regulators to ensure there are no misplaced concerns about its use. Its development should be continued throughout Phase 2, with the intention that it can be fully signed off for use as the regional simulator in Phase 3 and beyond (Section 5.2). It would however unlikely be available as a full regional simulator in time for the options identification and testing task in Phase 2.

No additional primary pathways were identified by the scoping team, but two suggestions were put forward during the water company interviews. The first was to phase model detail rather than functionality. This is a valid approach, but scoping showed that system detail is likely to be important from the outset to achieve satisfactory model performance; in particular, in the Thames catchment. The other suggestion was to focus model development on companies with the highest strategic needs or level of connectivity. However, it was clear from engagement with the companies that all are planning to integrate the regional simulator into their planning processes (in some cases water resources models have not yet been developed by companies), hence they will all require reliable outputs for their areas. Also, there would be limited gain from excluding or simplifying any smaller supply systems.

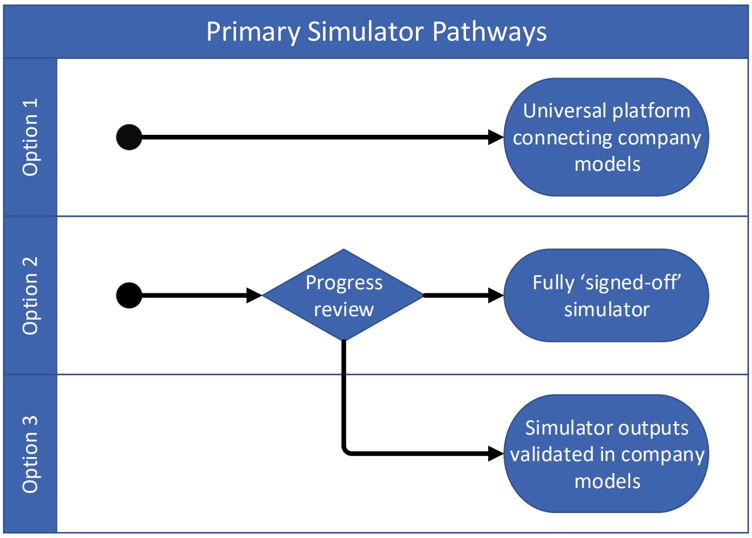


Figure 4-1 – Primary pathways considered

4.2.1. Feedback on the sign-off process

Following the issue of the draft scoping report Affinity and Thames Water provided comments in relation to the sign-off process and Plan B approach, as reproduced below.

Affinity Water comments

"It is mentioned in the draft scoping report that if the simulator cannot be fully signed off, a 'Plan B' is available whereby a reduced functionality simulator will be used alongside more detailed and accurate models owned by water companies. Rather than making a decision between building a full simulator or a reduced functionality simulator, we think that a decision needs to be made about identifying and agreeing what factors and criteria are critical to the development of the simulator. Therefore, the key aspect here is not what to include in the simulator but what criteria and factors the group would like the simulator to be calibrated and validated against and how well it can reproduce those factors considered as 'must-do'. Following this approach, the elements already identified as having high priority in the draft scoping report can be further prioritised using a traffic light system based on what water companies think the most important criteria for calibration and validation are. This could allow a graded approach, where criteria are 'dropped' in a managed way as the simulator build and validation progresses if required. We think that the identification of the key validation and performance requirements, by company, needs to form an urgent first stage of the Phase 2 work."

Thames Water comments

"… we've got a number of our comments … that relate to the programme and decision-making around developing a full simulator (Plan A) or a reduced functionality simulator (Plan B). At the moment, the process set out in the draft report around the decision-making is not sufficiently clear, with the implications for companies of the reduced functionality simulator (Plan B) route needing to be clearly spelt out. As we noted in our comments following the conference call… the need to implement Plan B brings with it a significant regulatory risk, with potential differences existing between the regional model and individual company models and misalignment of Preferred Programmes of investment that might result. We will need to ensure that we consider the risks and plan for dealing with them should Plan B be the outcome."

Taking this feedback onboard, an early start task has been identified (subject to agreement with WRSE) to discuss and agree with all stakeholders the full sign-off process. The task will involve the following steps:

- Building on the tender document, the scoping workshop outcomes and the report feedback, discuss and agree a clear testing and sign-off procedure for Phase 2, including reviewing the need for a 'Plan B' approach (including any regulatory considerations), and the decision points which would trigger a move to Plan B.
- Meet with companies to discuss and agree the specific performance metrics to include within the simulator testing framework.

If the early start task is commissioned, then workshops will be planned to provide all members of WRSE with the opportunity to shape and agree the final approach. The outcomes will be reported as an addendum to this scoping report. If the early start task is not commissioned, this would be a critical task to deliver at the commencement of Phase 2.

4.3. Modelling platforms – broad assessment

In the initial modelling platform assessment, a range of potential software packages for the regional simulator were reviewed against criteria representing the general requirements of the WRSE simulator (Table 4-2). The results of the assessment are shown in Table 4-3 and for those packages that were not taken forward for more detailed assessment the reasons for their exclusion are presented in Table 4-4. A full description of each package is included in Appendix C.

Of the nine platforms tested, six (Miser, Wathnet, IRAS-2010, WEAP, Source and RiverWare) were assessed to have significant drawbacks in terms of suitability (red cells in Table 4-3). Kestrel-WRM did not have any significant drawbacks but the software provider expressed the following reservations on its suitability and development as a regional simulator; "whilst Kestrel-WRM is functionally capable of meeting the WRSE objectives, the timeframes would make its use from scratch for WRSE, along with developing any necessary supporting infrastructure (e.g. GUI) very challenging and other solutions may be better placed. It is also unproven at the regional scale."

Aquator and Pywr were therefore taken forward to the detailed assessment (Section 0).

Table 4-2 - Broad assessment selection criteria

Criteria	Description
Runtime	To run large stochastic datasets across multiple scenarios it is important that the simulator has a fast runtime. A fast runtime also increases the scope for adding additional complexity to the simulator while still allowing more advance modelling techniques to be applied.
Flexibility	Adding innovative new functionality that WRSE needs to the modelling platform requires that either; • The platform is open-source allowing the source code to be directly modified. • The platform includes an Application Programming Interface (API) detailed enough to allow complex functionality to be added. The model owner takes primary responsibility for all simulator developments for WRSE.
Usability	WRSE and the companies want to be able to use and modify the simulator themselves. Modelling platforms that have mature and familiar interfaces have an advantage in this criterion. Good documentation and training material are also important.
Cost / Licence restrictions	Restrictive and expensive user licences are seen as a disadvantage, as each company would need to purchase them. Restrictions and or additional cost for running the model in parallel on the cloud are also a disadvantage.
Features	Some functionality such as the ability to model bidirectional links and the ability to include financial costs are essential. Others such as inbuilt DO analysers will help minimise development time.
Track Record	A record of being successfully used within the UK water industry, especially for large complex models, is seen as an advantage.

Table 4-3 - Summary results of broad assessment

Criteria	Aquator	Pywr	Kestrel	Miser	Wathnet	IRAS-2010	WEAP	Source	RiverWare
Runtime									
Flexibility									
Usability									
Cost/ licence restrictions									
Features									
Track Record									

Table 4-4 - Broad assessment software exclusion justification

Platform	Primary reasons for exclusion
Miser	• Expensive and restrictive licensing • Runtimes potentially an issue • ‘Black box’ optimisation process
Wathnet	• Limited inbuilt functionality • Cannot represent bidirectional links

IRAS-2010	• Limited ability to model complex operating rules • Difficult to modify (any changes have to be made directly to the source code) • Limited support available
Kestrel	• Not proven at a regional scale • Too much development needed for project timeframes
WEAP	• Licence cost • Not able to represent complex operating rules • International model not widely used in UK
Source	• Expensive licence and support • Lack of information about runtimes • International model not widely used in UK
RiverWare	• Expensive licence and support • Lack of information about runtimes • International model not widely used in UK

4.4. Modelling platforms – detailed assessment

In the detailed assessment the suitability of Aquator and Pywr was tested against each of the specific prioritised functionality requirements. The results are shown in Table 4-5; green shading indicates where one platform has a significant advantage over the other.

Table 4-5 - Modelling platform detailed assessment results

Criteria	Priority	Aquator	Pywr	Summary
F1. Runtime	High	• Aquator XV is faster than the previous version of Aquator but speed can still be problematic when running large stochastic datasets through complex systems. • Work is being carried out by HLS to improve speed but there is no specific timeline for this. • XM can run multiple instances of Aquator concurrently which can reduce runtimes in some instances, though this can have cost implications.	• Pywr has been developed to have the speed to easily deal with large stochastic datasets. This was directly due to difficulties experienced using Aquator. • Performance has been demonstrated on projects such as WRSE and WRE. It is relatively easy to parallelise Pywr on cloud platforms or multicore machines. • Benchmarking conducted by Atkins has shown that Pywr is significantly faster than Aquator on a like-for-like basis. • At each timestep, Pywr uses the GNU Linear Programming Kit (GLPK) (https://www.gnu.org/software/glpk/) to optimise the allocation of water. GLPK is an open-source software package that solves integer and mixed-integer linear problems using the revised simplex method. In benchmark tests, GLPK has shown to be one of the better performing open-source linear programme solvers. Pywr has previously been coupled with the lpSolve package (http://lpsolve.sourceforge.net/5.5/) and other solvers, including commercial ones, could be added in the future. • Some commercial solvers such as Cplex are considerably faster, however the licence costs are very high and could be prohibitive in this case. As a rough guide, the increase in model runtime due to complexity is considered to be approximately cubic. We were unable to find any evidence that this relationship was altered by using faster solvers. Utilising the speed of a commercial solver in Pywr does nevertheless provide a viable (but costly) way to combat increasing model complexity. At this stage however a commercial solver is not considered to be a likely requirement. • The United Utilities Strategic Resource Zone model has a similar level of detail and complexity to WARMS2. The Pywr model contains around 80% of the detail of the Aquator model but is around 100 times faster (Aquator v4.3). Further gains are achieved when multiple scenarios are simulated simultaneously. Pywr processes them all within the same allocation procedure, whereas Aquator runs them in parallel, but as separate instances. Up to a point, the more scenarios that are run, the higher the gains are. • In other testing performed for United Utilities, using the exact same configuration (including 500 years of stochastic data), automated optimisation of a reservoir control curve took 6 days in Aquator (v4.3) and 4 hours in Pywr. The Aquator optimisation module is not currently available for XV but running the same model in normal XV simulation mode was around 4x faster than v4.3 (Hydrologic quote an improvement of around 3x faster).	Tests have shown that Pywr has a significant advantage in terms of runtime
F2. Timesteps	Moderate / High	• Aquator is designed to run on a daily timestep.	• Pywr is designed so that it can be run on multiple different timesteps. • Input timeseries are automatically resampled to match the selected timestep length. • However custom operating rules would need to be manually adapted.	Pywr has the flexibility to vary timestep length.
F3. Option identification and optimisation	High	• Aquator interface provides a good tool for manual identification and testing of options. • GA3 module allows for automated optimisation using an MOEA.	• Manual option testing can be carried out similarly to Aquator, but this would be using scripts/notebooks rather than a GUI • Pywr has inbuilt optimisation functionality. Linked to 3 optimisation libraries that include various MOEA algorithms.	Aquator interface gives it some advantage in terms of manual testing but Pywr's speed and flexibility make it much more suitable for the application of MOEAs and other automated optimisation techniques.
F4. Adaptability to different conditions	High			Both Aquator and Pywr can represent complex operational rules and both use a similar optimisation process for the allocation of water during each timestep
F5. Outage Modelling	Low	• It is relatively simple to set Aquator up to run outage scenarios.	• Pywr does not include any specific functionality for outage modelling but it would be relatively straight forward to carry out simulation of outage scenarios.	If a Monte Carlo approach then Pywr's speed would be an advantage
F6. Option/ portfolio testing	High			Both Aquator and Pywr have the functionality to test the performance of option portfolios, however Pywr's speed would be an advantage for testing stochastic inputs over many scenarios.
F7. Deployable output	High	• Aquator is widely used to calculate DO and has inbuilt functionality to do so. • Used by many of the WRSE companies for this purpose.	• Pywr does not have inbuilt functionality but DO can be calculated using relatively simple scripts. • This was demonstrated with the current WRSE simulator to calculate stochastic DO for two of the sub-models.	Aquator's inbuilt functionality gives it the advantage over Pywr
F8. Dynamic groundwater	High	• Aquator does not include functionality for dynamic groundwater. • Adding it would probably require changes to the source code and therefore require input from Hydro-Logic (they are looking at this but have no firm timeline yet).	• Pywr includes the functionality needed to represent dynamic groundwater in the form of 1D and 2D polynomial parameters.	Irrespective of the selection of Aquator or Pywr, the majority of work required will involve building empirical models outside of the simulator. However, Pywr has the advantage in that it already includes the functionality to incorporate these models and would deal better with the extra complexity in terms of speed.

Criteria	Priority	Aquator	Pywr	Summary
F9. Water Quality	High / moderate			Both Aquator and Pywr can easily include WQ defined constraints but both would need significant development to model WQ directly (Pywr more flexible in this sense).
F10. Operational drought modelling	Low	• Aquator is widely used for this purpose and has in-built risk analysis tool	• Pywr does not include specific functionality but it would be relatively easy to carry out operational drought modelling. In the case where stochastics is used then Pywr's speed is an advantage.	Aquator usability and track record gives it an advantage though Pywr's speed may be beneficial where stochastics is used.
F.11 Natural Capital	Low			Not a priority at this stage. Both Aquator and Pywr could be used to extract metrics to inform natural capital analysis
F12. Multi sector representation	Moderate			Initially, both Pywr and Aquator can easily deal with this. However, if the complexity of multisector representation increases in the future then Pywr's speed becomes an advantage.
F13. Visualisation	High		• More efficient if using a Python visualisation platform	Will be primarily developed outside of the modelling platform so software package not a significant factor.
F14. Usability	High	• Aquator has a well-established GUI that is well known in the UK water industry. VBA scripting means that it possible to define complex operating rules (although requires coding skills).	• Pywr does not have an open-source GUI, though Manchester University have developed a web-based interface. Pywr models are primarily built and run using Python scripts and/or notebooks. Python is a simple and powerful programming language that is now among the world's most popular, which is potentially a benefit in terms of resourcing. • It is envisaged that water companies would not need to use Python to run the model, but some further development is required to get to this point.	Aquator's familiar GUI gives it an advantage in terms of usability however Pywr's Python interface is flexible and powerful, and GUIs are being developed.
F15. QA	High	• XV saves previous versions of the model but the QA functionality for custom VBA code within Aquator is quite limited, in terms of functionality and usability.	• As Pywr is a python library it is easy to use a version control system, such as Git, to track development, add unit tests, and carry out code reviews using a platform such as GitHub. Continuous integration could also be used to automate some of this process.	Pywr will allow a software development approach to be taken to QA (unit testing, code review, version control, etc.) which would be more robust than Aquator's internal version control system. This approach will also be easy to integrate with the QA of other workstreams.
F16. Data Management	High			Will likely be dealt with externally to the modelling platform.
F19. Bidirectional links	Moderate	• Has bidirectional links but some issues in use. Therefore, often represented as two links and this does not always work that well.	• Cannot be modelled directly but can be represented by using a two links and assigning some cost to their use, which avoids a circular flow of water between the two nodes.	Generally represented in both models in the same way.
F20 Inter-regional transfers	High			Should be straightforward in both Pywr and Aquator.
Licence costs/ restrictions	Moderate	• Costs associated with purchasing licences for XV and XM (for running multiple instances).	• Pywr has a GNU GPL v3.0 open-source licence. This means there is no licence cost and there are very few restrictions on it use.	No cost and limited restrictions on use give Pywr the advantage
Flexibility	High	• It is not possible for users to modify Aquator's source code but using VBA it is possible to add extensive functionality. However, Hydro Logic could modify Aquator to include new functionality given sufficient time and budget.	• As it is open-source, Pywr's source code can be directly accessed and modified. The code has been developed so that it easy to extend Pywr's functionality by building on existing Python classes and methods. Pywr can be run on Windows, Linux or Mac OS operating systems.	Pywr is more flexible as the source code can be directly modified and extended. It is also easy to run Pywr on different operating systems and the cloud.
Hydrology	High	• Rainfall run-off models can be effectively embedded into Aquator through customisation, as demonstrated by Thames Water's WARMS2 Aquator model. Its bespoke rainfall-runoff models are well calibrated to flows at Teddington.	• Pywr can be closely coupled with PyCatchmod and other rainfall-runoff models.	Complex hydrology can be represented effectively in both packages. The speed of Pywr means that doing so has less of an implication for run time.
Translation from existing models	High	• With exception to South East Water's Kestrel-WRM models, all existing resource zone level behavioural models for the South East are developed in Aquator. It would be easier to port them to an Aquator rather than Pywr regional simulator. In terms of replicating the structure this would not be a large saving. However, some of the complexities and customisation, for example contained in the Thames catchment models, would take additional effort to transfer to Pywr (simply because any VBA code would need to be rewritten in Python). Where the existing models are still in Aquator v4.3 they would first need to be converted to Aquator XV. This step would be required at some point but it is non-trivial (especially for VBA customised models) and would take up significant time in the Phase 2 development window.	• The previous WRSE model is already created in Pywr. It's clear from scoping that a different model structure would be required in some areas, however a significant proportion of the structure could likely be retained. Also, the connectivity between companies has already been modelled in Pywr, plus there is a separate Pywr model for the Havant Thicket reservoir option.	There are advantages to both; Pywr because the existing WRSE model provides a regional starting point and Aquator because the company models contain the additional detail / complexity that is likely to be required. Conversion from v4.3 to XV would create a significant programme risk, especially if there were issues with the conversion.

Criteria	Priority	Aquator	Pywr	Summary
Resourcing / training	High	• Aquator is a much more commonly used model and it requires less training for a user to become competent. Therefore, at this point in time at least, there are significantly more Aquator modellers. At the same time, there are many more Aquator models and therefore modellers are committed, and generally in short supply. Due to Aquator's usability the training of new modellers requires less effort. • However, any complex modelling – as would be required for WRSE - still requires programming skills (VBA). This aspect is no less difficult than using Pywr with Python.	• There are far fewer Pywr users, although the number is growing as the software becomes established. There is an active UK user group and an international user base. A small number of water companies have already embedded the software into their planning activities. Due to the nature of the software, it is more difficult to train a Pywr modeller at present but user interfaces are in development and the open source nature of the software means it is accessible to anyone with the requisite skills.	Whist the number of Pywr modellers is growing, Aquator has the advantage here due to the size of the existing userbase and the ease of training new modellers. However, the gap is likely to narrow over the coming 1-2 years and using Aquator in this type of application requires advanced modelling skills anyway.

4.5. Recommended simulator pathway

As set out in Section 0, both Aquator and Pywr have a high level of suitability for most of the individual requirements. The main limiting factor is that when the requirements are considered in combination, run speed becomes critical. For this reason, Pywr provides the best functionality needed for Phases 2 and 3. The advantages that it has in this area will also permit the development of some of the additional functionality desired further into the future, such as the automated optimisation of control rules and transfer options.

Even if Aquator was fast enough there is insufficient time in the Phase 2 programme to develop some aspects of the required functionality. The existing WRSE Pywr regional simulator provides a helpful starting point in this respect, and much of the required functionality has already been implemented elsewhere in Pywr, for example the lumped parameter groundwater modules embedded into the WRE regional simulator.

The main drawback of Pywr is that it is comparatively less user friendly than Aquator, considering the primary water company practitioners who will run the model. Whilst it will be possible to significantly close the gap, there is a limit to how much of this can be achieved in the short window available in Phase 2. Significant development can be undertaken in the medium term and the user interface can be specifically tailored to the companies' needs. Time has been included in Phase 3 to ascertain the specific requirements and put a firm development plan in place. A visualisation tool developed in Phase 2 will allow the companies to easily understand the model outputs right from the start, both in terms of headline results and detailed model operations (e.g. simulated transfer flow over time). This position is summarised in Table 4-6.

Table 4-6 - Plans for embedding the simulator into water companies

Phase	Exploration of model outputs	Ability to run the model	Responsibility to undertake runs during this phase
2	Visualisation tool	Using Python code only*	Consultant
3	Visualisation tool	Using Python code only. Scoping of interface design undertaken in this phase.	Consultant
4 (outside the scope of this programme)	Visualisation tool	Develop / adopt interface with high level of usability	Companies / consultants
Long-term	Visualisation tool	User interface	Companies / consultants

* Note that data security / access privileges (i.e. relating to individual company data) will need to be addressed before the model can be transferred in any form.

5. Simulator development

5.1. Approach

Assuming there is sufficient resource, all of the functionality mentioned in this document, through to fully automated optimisation of transfers, water quality modelling and regional Monte Carlo outage assessments, could be implemented for WRMP29 (WRSE26).

For WRMP24 (WRSE21) - Phases 2 and 3 - there are a large number of high priority requirements to be met. The length of the available development window presents challenges in terms of delivering this functionality. The following sections set out what should be possible in the time available for Phases 2 and 3 (assuming these phases can be commissioned in a timely manner) and sets out a road map for development in future phases.

5.2. Development road map

Figure 5-1 provides a high-level overview of the development road map. Initial tasks between Months 1 and 4 lead to a decision point on whether a regional simulator or reduced functionality simulator is possible. The road map diverges in the Months 5 to 9 depending on that decision. Results from the simulator produced in the option identification and testing process could feed directly into the investment modelling work. With a reduced functionality simulator, these results would need some testing and sign-off from the companies using their own models, with direct use of the company models providing an ultimate backstop. In parallel, the reduced functionality simulator would continue to be developed so that it could be signed off as a full simulator for Phase 3. Phases 2 and 3 encompass the development of all the functionalities in Table 3-2 and their incorporation into an integrated modelling platform that is accessible to all the WRSE companies.

The figure is intended to show the process at a high level and does not include every possible link between the tasks and tools. It is proposed that the approach to simulator sign-off and a ‘Plan B’ approach be further discussed and finalised in an early start task, as outlined in Section 4.2.1.

5.3. Programme

Figure 5-2 is a Gantt chart showing the development programme through Phase 2 and 3 for ‘Plan A’. A detailed programme for ‘Plan B’, which would cover the same timeframe, is not included at this stage but will be discussed as part of the proposed early start task, as outlined in Section 4.2.1. Several workstreams have been separated out from the core simulator development process, reflecting the fact that these could be carried out in parallel with the simulator build, and then integrated into the simulator at a later stage. These workstreams include: dynamic groundwater, hydrology, visualisation and dynamic demand forecasting.

A separate column shows specifically which tasks across the programme could be undertaken by parallel teams. Where this column is marked it indicates that the task could feasibly be completed more quickly by increasing the level of resources. It should be noted that this could in turn decrease overall efficiency for this work package and therefore increase the overall cost. It could also introduce additional risks from a quality assurance perspective. Where this column is not marked the task needs to be undertaken as part of the core model development over the time period specified in the programme.

In summary the key areas that need to be undertaken by the core development team (i.e. those that are time critical) are the ones that relate to the underlying simulator source code / architecture. The main modelling opportunities to use additional resources to reduce programme length (i.e. resource critical) are in developing the simulator structure, i.e. the representation of the supply system, and performing model runs. However, competence in the Pywr software would be required as a minimum level of capability. Separate tasks such as developing lumped parameter groundwater models or water quality constraints can be undertaken completely offline from the simulator development process, albeit following a specification for incorporation into the simulator. Some tasks which at face value might appear relatively distinct from the core development process, for example the visualisation tools, will likely produce much higher quality outputs if they are developed in conjunction with the architecture of the simulator.

Figure 5-1 – High-Level Development Roadmap

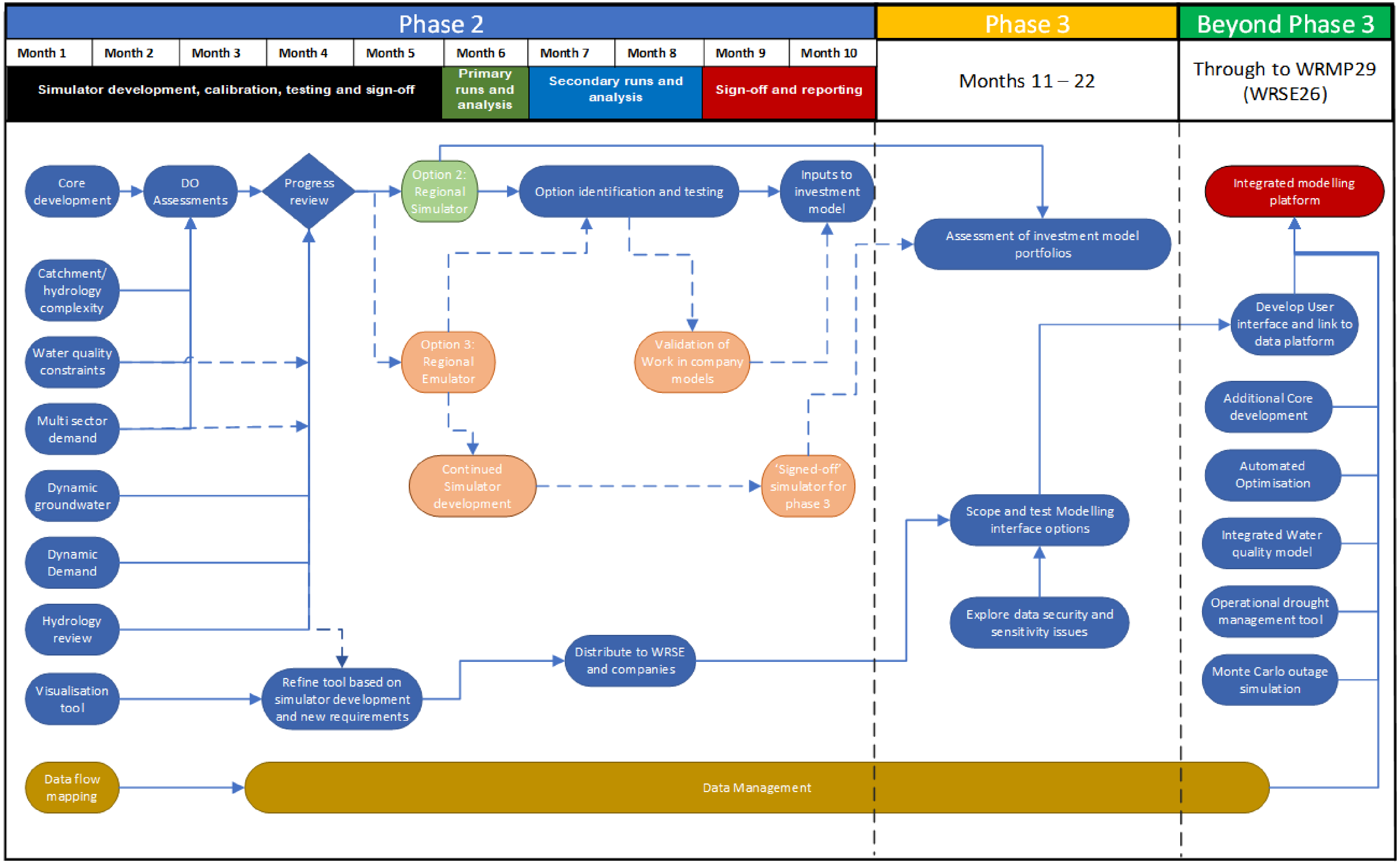


Figure 5-2 - Development Programme

5.4. Indicative time inputs and costs

5.5. Risks

A number of risks have been identified and set out below, along with some recommended mitigation actions. The list is not intended to be exhaustive but includes some key points that arose during and following scoping.

5.5.1. Procurement timing

The timescales for the procurement of Phases 2 and 3 are not yet confirmed. For scoping it was assumed that procurement would be concluded during September 2019 with a projected start date of 1st October 2019. As the start date has passed at the time of writing, the programme (Figure 5-2) is now structured around month number from a future start date. The length of the programme is driven by the tight original delivery timescales, and in all likelihood could take longer. As the programme is already very condensed any delays to the starting point could affect the delivery points of Phases 2 and 3.

To help mitigate any potential delays we have identified a number of early-start tasks that could potentially be undertaken separately to the main contract to help to keep the programme on track. These are highlighted in the programme (Section 5.3) and listed below:

- Produce a dataflow map showing how data and information will pass between the different WRSE tools / work packages including this simulator, the investment planning model, the options identification process and an overarching data management system.
- Agree simulator performance metrics and the sign-off / 'Plan B' approach with stakeholders
- Collate and review the existing input data
- Define and develop the model architecture to allow rapid development of regional model at commencement of Phase 2, and conduct review of existing regional PyWR model functionality
- Conduct the vulnerability assessment and prioritisation of groundwater blocks
- Acquire and review company groundwater models
- Acquire and review company models and identify any issues or areas where complexity might be required (e.g. Thames catchment)
- Set out the detailed approach for calculating DO for the supply forecasts and options benefits
- Start scoping suitable visualisation tools / libraries and review visualisation requirements with the companies, as well as interfaces with other workstreams

5.5.2. Input data checks

The performance of the regional simulator will be checked against company models using consistent input data, for example the companies' historic inflow data and modelled demands. Following sign-off some of the company model sourced data will be updated to regional data, for example spatially coherent stochastic inflows, or with new functionality such as groundwater simulation or dynamic demand.

Where relevant to the regional simulator a review of the company models and tools that have been used to help generate the regional input data (e.g. rainfall-runoff models) has been requested. This review may highlight the need to update some of these models and tools, although this could have additional programme implications. Also, irrespective of this using the regional input data in the simulator will likely alter the model outputs relative to the water company models, in some cases materially. Time has been allowed in the programme to allow this review process and, crucially, to work through any findings with the relevant water company.

5.5.3. Additional risks

As emphasised above, the model build programme is both ambitious and tight. Validation and sign-off will all be subject to inevitable model build uncertainties. This will need careful programme management and review and consideration of trade-off of required functionality, perhaps deferring higher risk development into Phase 3.

The development of lumped parameter groundwater models as well as delivering the desired catchment hydrological integrity are key risks given the complex nature of many of the catchments, and the approach to prioritising catchments / groundwater units suggested here (section 5.7) should help to mitigate this risk.

5.6. National modelling

The scoping review looked at whether there are any aspects of the ongoing national modelling exercise, led by the Environment Agency, that could influence the development of the WRSE regional simulator. Due to differences in approach, particularly with respect to the nature of the input data, nothing significant was identified to pass across at this stage. However, regular review of the national modelling in this context is recommended. It was noted that the National Modelling project is due to report in December 2019, and this will require review of the key findings and outputs and their relevance to WRSE.

5.7. Groundwater assessment framework

As recorded in Table 3-2 the dynamic representation of groundwater and surface water interaction is seen as an important functionality of the simulator in some areas of the region. Due to complexity and runtime issues the use of company groundwater models within the simulator, or directly linked to the simulator, was ruled out.

It was agreed that companies undertake a vulnerability/risk assessment of their groundwater blocks early in the simulator build phase to prioritise development and inform representation of those prioritised groundwater units in the simulator. The framework to undertake the vulnerability/risk assessment will be defined and coordinated by the simulator development team with the approach discussed and agreed with water company specialists. A number of risk factors will be assessed for each aquifer block (or this could be focussed at source or WRZ level), such as:

- Level of surface water – groundwater interaction
- Risk of abstraction exacerbating environmental deterioration
- Risk from saline intrusion
- Sensitivity to drought
- Availability and nature of existing groundwater models

Aquifers blocks will then be mapped to a suitable approach. A number of methods were proposed during scoping, ranging from:

- DO profiles
- DO timeseries based on relationships with hydrological input data, for example linked to drought indices
- River gravel abstractions / shallow aquifers to be treated as run-of-river surface water abstractions
- Lumped parameter groundwater models

Subsequent to the scoping exercise and workshops, Affinity Water proposed an alternative to a lumped parameter model which can be summarised as follows:

- Introduce groundwater DO algorithms with factors, set by WRZ, that will allow input groundwater level timeseries to be translated into average DO, peak DO and (if required) minimum DO. These values will vary by year depending on the groundwater level timeseries, coupled with volumetric constraints that limit abstraction during the summer period.
- For this approach groundwater levels will also be required for simulator runs involving stochastic / climate change influenced hydrology. Where feasible, run the full stochastic / climate change hydrological datasets through the groundwater models to determine the corresponding groundwater level. Where this is infeasible (due to run time), run a subsample of the hydrological dataset through the model and then build up a full record by interpolation based on the modelled recharge.
- Evaluate the impact on surface waters through simple relationships between abstraction reduction and flow-duration curve response.

Also worthy of specific consideration is that Thames Water's WARMS2 Aquator already contains lumped parameter aquifer units in which abstraction influences simulated aquifer storage and baseflow. However, it does not then link available abstraction yield to aquifer storage (simulated abstraction is based on a DO prolife).

The content of the framework should be set out, agreed and undertaken as a priority in Phase 2 or as an early start task (Section 5.3). It will be important to have a clear and auditable way of mapping each groundwater block to the different possible representations in the simulator. As noted by Thames Water, this is particularly crucial in terms of explaining why the representation of more complex interactions is not required. Much of the evidence needed is already captured in the conceptual models that underpin both numerical models and CAMS policy.

5.8. Deployable output

As noted in Section 1, subsequent to the scoping workshops and issue of the draft report the requirement to calculate DO was expanded to include supply forecasts and option benefits for investment modelling. Taken at face value this is a substantial volume of modelling work, although the associated simulator functionality development requirements would be fairly limited. DO runs are inherently time-consuming because they are iterative and difficult because they involve stretching the system to its limit and ensuring that it fails in a sensible / realistic manner. When the process also involves introducing new scenarios to the model such as stochastic droughts, climate change and different system configurations, extensive tweaking of model setup is often required, particularly where operational rules have been derived using historical conditions. This high level of human intervention means that it will be difficult to automate the overall process.

However, there are ways to reduce the workload here, for example by screening options to include in the analysis and inferring some results from other DO tests. Even with these steps in place at least one to two months modelling work should be allowed. This would impact on programme length and / or the ability to undertake other modelling runs and / or incorporate other aspects of simulator functionality.

Therefore, an early start task is recommended involving the following steps:

- Agree the time available in the programme to undertake this work
- Scope and agree the number and type of scenarios and options for testing
- Set out an approach for screening options (working with the options appraisal workstream)
- Set out an approach for inferring results from other DO tests

A workshop will be required to discuss and agree the approach with WRSE, and it is proposed that the outcomes will be outlined in an addendum to this report.

5.9. Hydrological analysis

Separate to this exercise a scope of work has been produced by WRSE outlining the hydrological analyses required to prepare input data for the simulator. This is included in Appendix D, for information. Note that the groundwater elements outlined in the document (numbered 4-5) could be developed as part of the groundwater assessment framework (Section 5.7).

6. Conclusions

The scoping review has drawn the following conclusions:

- There are a range of requirements for the WRSE regional simulator, many of which are technically challenging and high priority.
- Taking this into account, the development window for Phases 2 and 3 is relatively short.
- A fully signed-off regional simulator should be the main objective. If the simulator cannot be fully signed-off it could be used alongside the water company models as a reduced functionality regional simulator. The final sign-off process and approach to 'Plan B' could be discussed and agreed as an early start task and issued as an addendum to this report.
- The simulator pathway assessment found that Aquator and Pywr were the most suitable model platforms. Pywr was selected primarily because the run speed of Aquator would not allow the required functionality to be achieved.
- Work is needed to improve the usability of Pywr to the point where water company practitioners can run the model in-house, without Python programming skills. This work has been planned for beyond Phase 2, starting with a scoping exercise in Phase 3. Excellent visualisation of model outputs and model run operations is required in Phase 2.
- The development road map (Figure **5-1**) shows how the different steps fit together and the potential future developments beyond Phase 3, right through to WRMP29 (WRSE26).
- A number of programme risks have been identified. One risk is that procurement of Phases 2 and 3 will take longer than has been assumed in scoping. A number of potential early-start tasks have been proposed to help mitigate this risk - focused on those tasks that are likely to be most time critical. Addendums to this

report will be issued subsequent to the completion of the critical early start tasks that have been identified (subject to being agreed and commissioned by WRSE):

- Agree simulator performance metrics and the sign-off / 'Plan B' approach with stakeholders. Review performance of existing WRSE regional PyWR model against acceptance criteria.
- Design and develop groundwater assessment framework (for water companies to apply to their groundwater sources).
- Define deployable output approach and requirements.
- Define and develop the model architecture to allow rapid development of regional model at commencement of Phase 2
- Development of key requirements for Visualisation – developing scope / architecture of visualisation needs/tools/libraries, review of approaches used elsewhere, interface with other workstreams.
- Data management – scoping potential for a universal solution for data management that supports the simulator, any visualisation tools, and the other workstreams.

Appendix A

Appendix A. Modelling Specification (draft)

Appendix B

Appendix B. Modelling platform summary

B.1. RiverWare

Overview
RiverWare (Zagona et al., 2001; http://www.riverware.org/) is a water resource system modelling tool based on Object Oriented Programming paradigm. Users can create water resource system networks from pre-specified network objects such as reservoirs, stream gauges, canals, etc. using Graphical User Interface (GUI). Each object contains data attributes ("slots") and methods attributes (e.g., evaporation, seepage, etc.) which the user selects. Data associated with a particular object can be displayed and edited. RiverWare contains a water right (water ownership) modelling feature where the "paper water" is tracked separately from the real water at each time step. A separate view in GUI is available to display the water right accounts on objects and their linkages. The tool also features a Multiple Run Management (MRM) utility that sets up and executes multiple runs automatically. Direct data connections map data directly from/to Reclamation's Hydrologic Database (HDB) USACE Data Storage System (DSS) and Excel workbooks. The Scenario Manager offers a what-if scenario framework in which specified input variables can be modified and specified output variables can be viewed. The output of the model includes the time series of all system flows, storages and water right accounts. Both input and output data are stored as ASCII text files. The choice of computational time steps ranges from 1 hour to 1 year.
Technical description (Algorithms, method used to allocate/route water)
RiverWare offers 3 solution methods: pure simulation, rule-based simulation, and optimization. The pure simulation mode requires user-defined input values such as reservoir releases, storage values, diversions, etc. for operations. The rule-based simulation mode uses logical policy statements (operating rules) interpreted at run-time to determine the flows, storages and diversions, based on their priority. Rules need to be expressed in the RiverWare specific language, RiverWare Policy Language (RPL), by using a built-in syntax-directed editor. The optimization mode uses a pre-emptive goal programming algorithm and mixed-integer linear programming (MIP) to optimize user defined objectives which are optimized according to their priorities. I.e. the highest priority objective is optimized first, followed by the optimization of lower priority objective with the solution of the higher priority objective assumed as a constraint, and so forth. The MIP solver is used automatically to linearize any non-linear variable at each time step. The optimization results can then be used to simulate storages, hydropower generation, etc. based on the optimal releases and these simulation results can be used to refine the optimization output in turn. RiverWare uses the commercial optimization library CPLEX.
Unique data requirements
• Pre-specified storage, releases, etc. values for pure simulation mode. • Operating rules defined in the RPL language for rule-based simulation mode.
Strengths
• Object-oriented GUI – ease of application set up • Choice of 3 different solution methods • Able to track and account for water rights • Automatic multiple runs • No need to assign relative weights for objectives in the optimization mode
Weaknesses
• Cost – both initial and maintenance • RiverWare specific rule interpreted language RPL less computationally efficient than compiled code • No GIS capabilities (georeferencing the schematic is not possible)

Potential for regional simulation
RiverWare provides relatively high flexibility both in terms of the simulation mode and the type of analysis that it can be used for. The GUI may speed up the complex regional model network set up and modification. The automatic multiple runs feature may be particularly suitable for scenario analysis. However, the lack of information about the model run-times makes it difficult to estimate the model's suitability for the regional planning. The custom scripting RPL language would require the user to learn it beforehand to be able to specify operating rules. The high licence and maintenance fees may prove excessive for its suitability to the regional planning problem.
Ownership/Licensing
RiverWare was developed and is owned and maintained by the University of Colorado at Boulder's *Center for Advanced Decision Support for Water and Environmental Systems* (CADSWES). The commercial licence with free first year maintenance and 2-hour user support costs $7,150 for single node use without an optimizer and $13,000 for a single node with the optimizer. (http://www.riverware.org/riverware/LicensingRW/index.html). The additional user support costs $130/hour.
References
Zagona, E. A., Fulp, T. J., Shane, R., Magee, T. & Goranflo, H. M. 2001. RIVERWARE: A GENERALIZED TOOL FOR COMPLEX RESERVOIR SYSTEM MODELING1. *JAWRA Journal of the American Water Resources Association,* 37**,** 913-929

B.2. WEAP

Overview
WEAP (Water Evaluation and Planning) (https://www.weap21.org/) is a generic model containing two sub-models that simulate the natural hydrological processes within a catchment and anthropogenic activities, i.e. system management. The former includes a conceptual rainfall-runoff model, an alluvial groundwater model and a stream water quality model. The latter is driven by water demand prioritization, supply preferences and environmental requirements. The optimization model applies a mixed-integer linear programming routine to maximize demand satisfaction based on the above-mentioned preferences, mass balances, etc. to allocate water. Users can choose a daily, weekly or monthly simulation time step. WEAP features a Graphical User Interface (GUI) for constructing, viewing and modifying the system and datasets. A schematic of the system can be created by adding objects from a standard palette and georeferencing these. Time series are imported using a CSV file. GUI also provides a Results View feature, where the simulation or optimization results can be viewed in chart or tabular form. Charts, tables and data can also be exported to Excel. Different model scenarios can easily be developed using the Scenario Manager feature of the GUI. WEAP provides a possibility to extend its functionality with user–defined variables and user written functions (in VBScript, JavaScript, Perl, or Python).
Technical description (Algorithms, method used to allocate/route water)
WEAP calculates mass balances for every node and link in the system at each time step assuming all flows occur instantaneously (no routing). Each period is independent of the previous one except for storage and soil moisture. Water allocation starts with prioritizing demand nodes as specified by the user (integer values from 1 to 99, highest to lowest priority, respectively), where multiple demand sites can be members of the same priority group. Only after priority 1 allocations have been made, priority 2 allocations are activated, and so forth. The same procedure applies to the supply preferences to define which source will supply a single demand. The algorithm iterates over each supply preference to maximize the demand satisfaction at each demand site. WEAP considers 4 zones of reservoir storage divided into flood-control, conservation, buffer and inactive zones. The conservation together with buffer zones represent the active storage while the flood-control zone is kept empty, i.e., the volume of water cannot exceed the top of the conservation zone. Rule curves defining the storage zones and releases/targets can vary in time.
Unique data requirements
• User-defined demand priorities • Rule curves to define storage zones and releases/targets
Strengths
• GUI interface helps to learn and use the model easily • Simple model code thanks to the linear programming approach • Scenario analysis functionality • Compatible with GIS
Weaknesses
• Licence cost • No built-in flow routing functionality (may be however hardcoded in by the user) • Not able to iterate within a time step or multiple time steps • Not able to optimize multi-period problems • Not able to provide rule-based simulation (operation rules are stylized and relatively simple) • No ability to simulate water rights

Potential for regional simulation
WEAP can simulate both hydrologic processes and a water supply system management. GUI interface together with the georeferencing capabilities may ease the building up stage of the regional model. Scenario analysis functionality may ease the scenario testing phase. However, as the model does not allow for rule-based simulation, the operation rules may need to be simplified reducing the model’s credibility for regional planning. The licensing cost required, although lower than for RiverWare, will result in additional cost requirements for the overall project.
Ownership/Licensing
WEAP was developed and is distributed by the Stockholm Environment Institute (SEI). The non-consulting licence costs $3,000 for 2 years, may be used by an unlimited number of users at one site and includes free upgrades and limited support. SEI needs to be contacted directly to obtain consulting licence.

B.3. WATHNET

Overview
WATHNET is an optimization-based generalized simulation model (Kuczera, 1992). It utilizes a network linear program (NetLP) to simulate the operation thus reduces the need to for defining explicit rules to guide water allocation. It uses the information about the current state of the system as well as forecasts of streamflow and demand to formulate the NetLP. The NetLP searches for the minimum cost solution for distributing water through a network of unidirectional links connecting supply, demand and transhipment nodes (Cui et al., 2011). WATHNET contains four modules: 1. EDNET, a mouse-based graphics interface to define and edit the system schematic 2. WATSTRM to stochastically generate hydroclimate data and manipulate large files 3. SIMNET that formulates NetLP, performs multi-replicate simulation and saves results 4. WATOUT, an interactive graphic interface to study the SIMNET output file WATHNET implements NETFLO, a simplex-on-a-graph code (Kennington and Helgason, 1980) which is able to solve a NetLP problem 100 times faster than standard simplex solver.
Technical description (Algorithms, method used to allocate/route water)
The NetLP (formulated by SIMNET) determines the water allocation (flow through the network links) in a single time step following a hierarchy of objectives: 1. Satisfy demand at all demand nodes 2. Satisfy all instream flow requirements 3. Ensure that the reservoirs are at their end-of-season targets 4. Minimize delivery costs 5. Avoid unnecessary spills The network is divided into three sub-networks to perform the simulation: the shortfall sub-network ensures the objective 1 is satisfied, the instream sub-network ensures the objective 2 is satisfied, and the storage carryover sub-network ensures the objective 3 is met. WATHNET offers two other algorithms to produce high-speed computation: RELAX (Bertsekas, 1992) that implements primal-dual algorithm with the ability to start search from a prior solution; and PPRN (Castro and Nabona, 1996) that can handle linear constraints and linear flow routing but is significantly slower in solving NetLP when compared to RELAX.
Unique data requirements
None
Strengths
• WATHNET is a fast model and utilises the advantages of a NetLP over the more standard simplex solver. • Graphical User Interface (GUI) • Built in tools for running multiple “replicates” (i.e. scenarios) of a model.
Weaknesses
• WATHNET has very limited built-in functionality. Even simple operational rules (e.g. annual licences) need to be written in code by the user manually. • Only simplified representation of a network • Only unidirectional links possible to represent (although cyclic structures are possible) • Routing only possible with the PPNR algorithm which is computationally more expensive • Not able to simulate hydrologic processes of a river basin

Potential for regional simulation
WATHNET is a very fast water resource simulation model and has good potential for application to the regional planning problem. However there are a number of issues that may inhibit its use. The lack of built-in functionality for common operational rules means that the model requires extensive manual set up even for simple networks which may complicate and prolong the building of the WRSE regional model.
Ownership/Licensing
WATHNET was developed by George Kuczera (University of Newcastle, Australia) and is available upon request. No licensing information for commercial use is available.
References
Kuczera, G. 1992. Water supply headworks simulation using network linear programming. *Advances in Engineering Software,* 14**,** 55-60.

B.4. Source

Overview
Source (https://ewater.org.au/products/ewater-source/ ; Welsh et al., 2013), also known as Source Integrated Modelling System (Source IMS), is an integrated planning and operations tool for catchments, rivers and their connected groundwater systems that can be used for urban water supply management at the town, city, and regional scale. It is able to address a variety of river management and operations aspects including catchment runoff, river flow routing, reservoir routing and releases, surface-groundwater exchange and conjunctive use, urban, ecological, industrial and agricultural demands, water quality, etc. Source sub-components include graphical user interfaces for model configuration (using node-link river network schematic), scenario management, data management, visualization and reporting. Graphical User Interface (GUI) allows building and modifying the network and run the software for user defined scenarios. The reporting tool allows post-processing of the results (graphs can be exported to a file or printed). Source provides flexibility to incorporate additional functionality, connect available plugins and connect the output of another model directly to the Source input. Simulation time step varies from daily to annually.
Technical description (Algorithms, method used to allocate/route water)
Source provides two simulation methods, rule-based and optimization-based. The former is able to model complex rules and processes, runs faster but does not search for the most efficient solution. The latter uses the NetLP linear programming to find minimum cost solution of allocating water through a network of links but can have longer run-times for complex networks, smaller time steps or longer travel times (Welsh et al., 2013). Reservoirs in both cases can be modelled both in parallel and in series where the latter are managed to minimize the spills, i.e. lower storage is used first to meet the downstream demands before the upper storage. Reservoirs in parallel can be managed in four different ways: 1. Independently, i.e. storage nodes release water based on the priorities 2. In harmony, i.e. storage nodes release water to balance the likelihood of spills 3. Order splitting, i.e. storage nodes release water as ordered by storage volumes 4. Access zones, i.e. storage nodes with a lower priority zone release water until the priority zones are equalized, then water is released in a defined ratio or harmony rules
Unique data requirements
• User-defined operating rules for rule-based simulation • User-defined type of operation for reservoirs in parallel
Strengths
• GUI provides ease of use • Flexible software infrastructure allowing the user to create and link additional functionality • Able to model hydrological processes as well as the water supply system management • Able to model routing, inter-basin management, agricultural and environmental demands, surface-groundwater interaction, water ownership and rights • Provides scenario analysis tool
Weaknesses
• Potentially expensive license • Longer run-times when using the NetLP method for complex systems with small time steps and lack of information about runtimes in general.

Potential for regional simulation
Source is able to model surface-groundwater interactions thus represent the surface-groundwater conjunctive use schemes effectively. Furthermore, it allows for inter-basin management and shared resource modelling making it suitable for regional planning. However, employing the optimization-based simulation in Source may results in extensively long run-times which may prove difficult for scenario analysis and/or optimization. The lack of licensing cost information makes it difficult to compare its availability to other available model software platforms.
Ownership/Licensing
Source was developed and is owned and maintained by eWater, an Australian government owned non-profit organization. It is available in two versions: a public version with limited functionality and free to download and use, and a full licensed version available as a single or discounted multi-copy licence (https://ewater.org.au/products/ewater-source/access-licensing/). There is no information available about the licence cost; to obtain a licence the user is required to email the eWater directly.
References
Welsh, W. D., Vaze, J., Dutta, D., Rassam, D., Rahman, J. M., Jolly, I. D., Wallbrink, P., Podger, G. M., Bethune, M., Hardy, M. J., Teng, J. & Lerat, J. 2013. An integrated modelling framework for regulated river systems. *Environmental Modelling & Software,* 39**,** 81-102.

B.5. Kestrel

Overview
Kestrel - WRM is a mass balance, node & link model similar to models such as IRAS-2010. Kestrel WRM is developed and maintained by HR Wallingford and model development & use has historical only been used in house. South East Water currently use Kestrel models that are run by HR Wallingford.
Technical description (Algorithms, method used to allocate/route water)
Demand allocation can be determined on the resource state of key nodes within the model (e.g. reservoirs) or using licence constraints and operational rules. Demand is allocated at a daily timestep however this could be altered through interaction with python source code. Python source code can also be interacted with to allow the addition of new features or model processes.
Unique data requirements
None
Strengths
• Potentially faster than models such as Aquator although unproven at WRSE scale. • Developed in Python and therefore functionality is flexible as code can be customised. • Can be dynamically linked to other external process models e.g. Kestrel - IHM (gridded hydrological model).
Weaknesses
• No GUI. • Untested at WRSE Scale. • Unused outside HR Wallingford so broader experience is severely limited.
Potential for regional simulation
Kestrel – WRM is functionally capable of meeting the WRSE objectives, however the tight timeframes would make its use from scratch, along with developing any necessary supporting infrastructure (e.g. a GUI), very challenging. It is also unproven at the scale of WRSE which creates uncertainty around run-time benefits.
Ownership / Licencing
Kestrel-WRM has not been used by any users except from within HR Wallingford and possible licensing arrangements have not been investigated. Although this is not seen as a barrier for models HR Wallingford have developed, for other model development and use an associated cost may be anticipated.

B.6. MISER

Overview
• Widely used for operational purposes, for example production planning, pump scheduling, outage and assessment of risk. • Used for water resources modelling (e.g. Wessex), although some companies use Aquator even if they have Miser for operational purposes (e.g. UU, STW). • Also used for investment modelling, but not extensively (?)
Technical description (Algorithms, method used to allocate/route water)
• MISER uses the EXPRESS-MP mixed-integer linear programming solver. • The model is solved using a list of user-specified priorities (e.g. minimise deficit, minimise cost, achieve minimum flows). The exact algorithm the model uses is unknown, i.e. a “black box”. • Has different optimisation time horizons: 80-100y, 50-20y, 1-2y and 24-168h. • Can conduct a ‘whole horizon optimisation’ (i.e. turn off the control rules), solve the model for each timestep, or solve using a sliding window.
Unique data requirements
None
Strengths
• Possible to run same model at different levels of temporal granularity and hence variable run-times. • Good functionality as a water resources model • Good reputation in terms of optimisation (but not sure of technical detail and often referred to as a “black box”) • Already includes EBSD type model
Weaknesses
• Expensive to licence and can experience difficulties around consultants using the software. • Can multithread but need buy a separate licence for each copy of the optimiser running (hence very expensive). • Inflexible in terms of customisation (but has good inbuilt functionality). Very difficult to get to inner workings. • Servelec working practices not conducive to research type projects, at least not without their full involvement. • Would be impossible to call the model from an external MCS routine – Servelec wouldn’t allow it.
Potential for regional simulation
It’s possible that MISER could be used for a regional simulation model but would need a lot of time and financial investment, and the majority of the technical work would need to be undertaken by Servelec. Even then run times are likely to be prohibitive.
Ownership/Licensing
The model is developed and licenced by Servelec – strict rules and expensive, as above

B.7. IRAS-2010

Overview
IRAS-2010 (Interactive River-Aquifer Simulation - 2010) (Matrosov et al., 2011) is a fast, generalised rule-based water resource system simulator. IRAS-2010 is a new code based on the original IRAS (Loucks et al., 1995) which was developed at Cornell University. IRAS-2010 models water flows and storages, single and joint reservoir releases, time-varying water consumption, abstractions and allocations, hydropower production and pumping energy use. The software is written in Fortran and is open-source allowing users to add new features or add customised operating rules. An IRAS-2010 model represents the system as a network composed of nodes and links of various types. Nodes can be diversions, natural lakes, reservoirs, aquifers, wetlands, gauge sites with a defined time-series flow, demand and consumption sites. Links natural or engineered flow paths between two nodes. IRAS-2010 uses text-based input files that define the system and its operating rules. The text-based output of the model includes the time-series of all system flows, storages and engineering performance metrics. Users can also hard-code custom output metrics. Users can choose a time-step ranging from 1 day to 1 year in day-long increments (e.g. a weekly time step is 7 days whilst a monthly time-step is 30 days). IRAS-2010 does not have a graphical user interface (GUI). IRAS-2010 is distributed as code and therefore can be run on any operating system including Linux. This allows the software to be connected to third-party evolutionary algorithms that can be run on parallel clusters. IRAS-2010 has been used in the proof-of-concept Water Resource of East WRE study which applied Robust Decision Making (RDM) and Many-Criteria Search to an infrastructure selection problem. It was also used for several Thames basin infrastructure selection studies which used RDM (Matrosov et al., 2013a, Matrosov et al., 2013b) and multi-criteria search (Matrosov et al., 2015).
Technical description (Algorithms, method used to allocate/route water)
IRAS-2010 is a rule-based simulator. IRAS-2010 is programmed in Fortran using procedural programming, meaning it organizes tasks into subroutines. IRAS-2010 requires user-defined operating rules (e.g. reservoir releases, storage values, allocation, and abstraction rules etc.). It does not utilise any optimisation algorithms to calculate allocations to demand nodes. Instead, IRAS-2010's internal algorithms break each time step into sub-time steps. IRAS-2010 adjusts demand-based reservoir releases and abstractions based on deficits in demand nodes based on previous sub-time steps. The number of time-steps is user-defined. The more sub-time steps there are, the more precise calculations become especially for complex systems. However, including more sub-time steps results in increased run-times. The user must therefore consider the trade-off between increased precision with more sub-time steps and the corresponding longer run-times. IRAS-2010 does not support scripting. Custom rules and features must be hard-coded.
Unique data requirements
• User-defined operating rules including reservoir release and abstraction rules.
Strengths
• Open-source (free to use) • Possible to customise the code • Fast runtimes (60-year Thames model runs in 1s using a weekly time step on a 3.5 GHz processor)
Weaknesses
• Does not provide a Graphical User Interface (GUI) • Source priorities cannot be explicitly defined • Use of sub-time step-based algorithm does not allow for complex operating rules (model cannot predict conditions at the end of a time step making rules based on modelled conditions difficult) • Use of bidirectional links is limited (e.g. bidirectional transfers cannot be represented) as upstream to downstream node calculation order is fixed

Potential for regional simulation
IRAS-2010 benefits from a fast and efficient code that results in quick model run-times. This allows it to be used in decision making frameworks that require thousands of model runs. However, IRAS-2010's limitations regarding complex operating rules and its inability to model bidirectional transfers may limit its ability to represent regional systems with many inter-connected subunits (e.g. water resource zones) and their operating rules with high fidelity.
Ownership/Licensing
IRAS-2010 is free to use and customise and is distributed with an open-source GNU General Public Licence V2 (see additional comments on the GPL in the Pywr review).
References
Loucks, D. P., Taylor, M. R. & French, P. N. 1995. IRAS - Interactive river-aquifer simulation model, program description and operating manual. *In:* CORNELL UNIVERSITY, I., NY. (ed.). Cornell University. Ithaca, NY. Matrosov, E. S., Harou, J. J. & Loucks, D. P. 2011. A computationally efficient open-source water resource system simulator - Application to London and the Thames Basin. *Environmental Modelling & Software,* 26**,** 1599-1610. Matrosov, E. S., Huskova, I., Kasprzyk, J. R., Harou, J. J. & Reed, P. M. 2015. Many-objective optimization and visual analytics reveal key trade-offs for London's water supply. *Journal of Hydrology,* http://dx.doi.org/10.1016/j.jhydrol.2015.11.003. Matrosov, E. S., Padula, S. & Harou, J. J. 2013a. Selecting Portfolios of Water Supply and Demand Management Strategies Under Uncertainty-Contrasting Economic Optimisation and 'Robust Decision Making' Approaches. *Water Resources Management,* 27**,** 1123-1148. Matrosov, E. S., Woods, A. M. & Harou, J. J. 2013b. Robust Decision Making and Info-Gap Decision Theory for water resource system planning. *Journal of Hydrology,* 494**,** 43-58.

B.8. Aquator

Overview
Aquator is a widely used conjunctive-use water resources model. Main role is calculating DO for WRMPs but use extends into drought planning, operational rules, asset management etc.
Technical description (Algorithms, method used to allocate/route water)
Aquator uses a linear-programming based solver (LP-solve) to solve the supply-demand balance on a daily timestep. The solver can function simultaneously to optimise costs and resource states. Depending on model setup any sources that have a healthy resource state (e.g. reservoirs being above their control curves) have their resources allocated on a minimal cost basis. When the resource state is poor the model is solved to maximise use of resources with a higher resource state in an attempt to balance resources. The solver does not support integer constraints (i.e. it is not a MIP). Aquator exposes an API via Visual Basic for Applications (VBA) which allows the user to write code to customise the behaviour of the model at different steps in the simulation algorithm. This gives the user a lot of freedom and allows the representation of complex operating rules. However, heavy use of VBA can significantly slow down model run times.
Unique data requirements
None
Strengths
• Graphical User Interface (GUI) • Good reputation – stakeholder confidence • Cloud functionality (with AquatorXM) which is capable of running, for example, 1,000,000 scenarios (however, the costs of renting instances of Aquator on the cloud would be significant) • Already used for RDM (Hydrologic resilience add-on) • Already used extensively with genetic algorithms (control curve generation with Exeter University) • Easy to build models with WRSE supply systems (e.g. Thames, Southern) already represented in Aquator - possible to simply copy model segments across. • Can be easily customised with VBA.
Weaknesses
• Processing speed? Even though AquatorXV is faster than the previous version the actual model calculation steps are still not multi-threaded (other things such as the GUI are). • To run 1,000,000 scenarios on 100 cores, and to rent Aquator instances, would cost ~£46.92 per hour and would require 10,000 sequential model runs on each core – which could take a significant amount of time (208 days) if a single run took ~1/2 hour. • Need to purchase licences for the software, XM, and rent instances of Aquator on the cloud to run large datasets.
Potential for regional simulation
• Excellent tool for regional simulation. However, in the context of WRSE run-time would significantly constrain the number of scenarios for RDM, and/or the length of hydrology datasets that could be run through the model. • In terms of MCS/scheduling there is no existing functionality to select options so this would need to be added. Aquator is easy to control from Excel but this may be another significant constraint on overall run-time (i.e. Excel talking to Aquator back and forth). Note that this is tackled in the new AquatorXM module could be used to manage running multiple scenarios on the cloud. • So Aquator focus on usability and system simulation could be too much of a constraint for MCS and RDM.

Ownership/Licensing
• Originally developed by Oxford Scientific Software (OSS) – but now owned by Hydro-Logic Services. • Open and relaxed approach to licencing (c.f. Servelec). • Support from Hydro-Logic Services.

B.9. Pywr

Overview
Pywr is a mass balance model designed to represent flow through a network. The model is not restricted to flow of a particular type; raw water, clean water and electricity can be simulated in a single model. The structure and state of the model are distinct from the algorithm used to route flow through the network. In theory this allows for different routing algorithms to be used by the model, however in practice only one has been developed so far.
Technical description (Algorithms, method used to allocate/route water)
Pywr is a mass balance model designed to represent flow through a network. The model is not restricted to flow of a particular type; raw water, clean water and electricity can be simulated in a single model. The structure and state of the model are distinct from the algorithm used to route flow through the network. The algorithm represents the problem as a linear programme. The flow from each input (which adds mass to the system) and each output (which removes it) via a unique route is assigned a variable to be solved. The problem formulation is similar to the algorithm used in Aquator, but has some differences; namely, the way in which flow in rivers is represented (as a first-class flow, rather than implicitly) and the way storages are modelled. The problem is solved in a single pass, searching for a least "cost" solution which meets the constraints of the model, where cost is the net benefit of transferring flow via a particular route including financial and other non-financial considerations (e.g. resource state). The model is solved for each timestep, dependent only on the inputs current state of the model (as opposed to "whole horizon" optimisation which solvers multiple timesteps simultaneously). The application is written in Python, with core elements written in Cython (an optimising static compiler) for performance.
Unique data requirements
None
Strengths
• Pywr is fast, free and extendable. • The model has been written from the beginning with performance in mind. This is significant given the number of timestep evaluations required for multi-objective optimisation and stochastic timeseries. • The liberal licensing of the model (GNU GPLv3) means there is no restriction who can run the model, or how many instances of the model can be run. It also means that the source code can be directly modified to add new features. • The model is independent of operating system and can be run equally well on a Windows-based desktop machine or a high-performance UNIX/Linux-based cluster (e.g. Amazon Web Services). • The model can output results in the HDF5 format, which is particularly suited for storing the large amounts of data produced by such runs.
Weaknesses
• The number of users familiar with the model is small. • There is not currently a Graphical User Interface (GUI).
Potential for regional simulation
Pywr has been proven as suitable for regional simulation in previous work for WRSE, as well as WRE. Pywr's speed means that it can run large stochastic datasets through complex models in reasonable timeframes, while its flexibility means that new features/functionalities can be added in response to project requirements.

Ownership/Licensing
Pywr is licensed under the GNU General Public Licence version 3 (GPLv3). The copyright is owned by Joshua Arnott, James Tomlinson, The University of Manchester, and Atkins. The GNU GPL (version 3) is a *strong copyleft* licence. More information about this can be found on the GNU website (https://www.gnu.org/licenses/gpl-3.0.en.html). Without going into too much detail this has a few implications: • No limitations on who can run the application, or how many instances of the application can be run. • If the application is distributed as a binary, the source code must also be made available. This does **not** mean that the water resource models developed need to be made available. • The application is distributed “in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE”. Note however that this is not usual in the licences of other commercial products.

Appendix C

Appendix C. Scoping tender document

Invitation to Tender: Scope the WRSE simulation model for WRMP 24

Water Resources in the South East

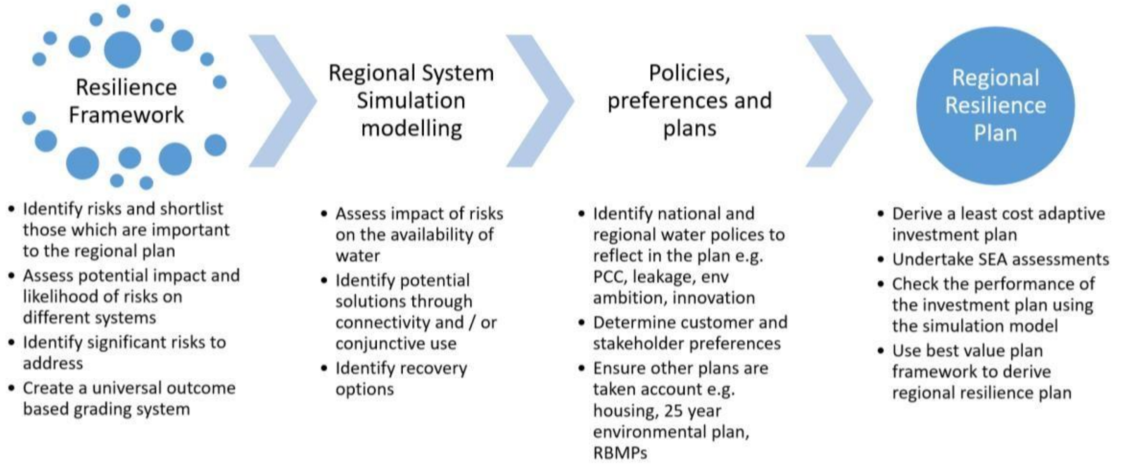
Project:	WRSE WRMP 24 regional plan	**To:**	Issued to Tender
Subject:	Scope the WRSE simulation model	**Created by:**	Meyrick Gough, PMB
Purpose:	To Tender	**Version, Date:**	Final, 04/06/2019

1. Summary

The purpose of this document is to invite bids to undertake the first phase of the regional simulation modelling work. This phase of work asks the consultant to review three potential ways, or more, in which WRSE could progress the regional system simulation modelling work and make a recommendation on which option is the best to proceed with.

2. Introduction

The six companies in the South East of England are seeking to develop a multi-sector, resilient water supply plan for the region by August 2021. To achieve this the group of companies will be developing four key areas of work, coupled with associated models, which will help provide the evidence to support the regional plan. The four areas of work are set out in the diagram below:



This invitation to tender is related to the second element of work, which is the regional system simulation model. Specifically, which modelling approach should the region adopt for the next phase of work.

The companies in the South East of England currently supply water to approximately 19 million people across ~31 water resource zones which have some, but limited, transfer capability as indicated in the adjacent figure. The mode by which systems are operated and the connections between the zones have evolved over time as different needs have occurred. The WRSE regional simulation model for PR24 should be robust and provide insights into how the system will cope with more severe droughts or other challenges in the future.

Currently the region has a mixture of simulation models on different platforms using different data. The purpose of this document is to invite bids to undertake a review of the current situation, the options, the PR24 programme and to recommend the optimal approach for the next regional system simulation model for the South East of England. This scoping is the first of two phases of work for the regional system simulation model. The second phase of work is the actual model development.

It is important that the simulation model can be used and maintained by the WRSE / member water companies, and not be reliant on third parties.

The tasks required for this phase of the work are:

1) Understand the extent to which a regional simulation model provides information to the development of the regional resilience plan (Appendices A-C) through interviews with key WRSE people and the Programme Management Board
2) Review the existing company and regional simulation models and their ability to be used to undertake the type of analysis that has been described in task 1
3) Based on the review (2) undertake an analysis of the additional development work required for these models in order to answer the questions that are being posed
4) Review and recommend, with indicative costs, which of the pathways WRSE could follow. This must consider existing models, potential data connectivity, challenges and opportunities versus the required outputs. The pathways are (but not exclusively):
    a. Option 1: Connect each of the companies' own simulation models together on a universal platform to allow the models to interact with each other
    b. Option 2: Improve the existing regional PYWR model to replicate the company's own simulation models and then use this model to undertake the simulation modelling approach
    c. Option 3: Hybrid approach. Improve the PYWR model different modes of operations and connections with a good degree of confidence. Then test the results of this work with the company specific models
5) Review and recommend how groundwater and water quality representation could be improved in these models by reviewing what companies currently do, and what data is available, in order to:
    a. Develop a series of options to improve the representation of groundwater in the regional and company specific models
    b. Discuss the various approaches and agree the most appropriate method for the chalk and sandstone blocks
    c. Provide evidence where these approaches have been used in the past.
6) Present the findings and the recommendations with WRSE & PMB in a half day workshop
7) Write a scope and draft programme for the development and running of the regional system simulation model(s). This scope will be used to invite tenders for the next, second, phase of the simulation work.

The deliverable for this work is a report that sets out the review undertaken, detailing the outputs of each of the above tasks. It must provide a recommendation for the modelling approach, together with an indicative cost for its development and operation.

3. Timescales

A timescale for the production of the next regional plan is still evolving but it is anticipated that the next regional plan will be produced by August 2021. In order to achieve these timescales and leave sufficient time to undertake the investment modelling work, scheme costing and multi-sectorial engagement, **all of the simulation development work must be completed by 31st March 2020**, i.e. model selection, build, calibration and validation and sign off.

Therefore, the timescale for this aspect of the work: *modelling scope* is as follows:

a) Invitation to bid issued 5th June 2019;
b) Tenders received by 28th June 2019;
c) Award by 12th July 2019; and
d) Final report (detailed, agreed specification) by 30th August 2019.

All bids will be assessed on quality of the bid submission, quality of the proposal, experience and ability to stick to deadlines. In the bid please make a provision to interview the WRSE companies and understand their existing models. Other useful sources of information such as the Pywr model review will be made available to the successful bidder.

4. Background information

The following points are provided to provide an oversight for the consultant:

1. **Company specific simulation models in the South East**: There are a number of water resource simulation models in the South East of England. These range from Aquator, Miser and Pywr through to some bespoke spreadsheet or other modelling platforms. Not all companies have simulation models and typically those that do have developed their models in a similar way but sometimes different ways. For example, some have rainfall runoff models included within them, other company models do not.

1. **Regional system simulation model**: WRSE recently (two years ago) commissioned and produced a regional simulation model in Pywr. This model has not been fully utilised by the companies in the region and still requires some further work to make it robust for use in a regional context, for example on groundwater simulation.
2. **Groundwater**: Whilst a number of the company simulation models summarise groundwater components within them, not all of them do. Also, the level of sophistication of this groundwater representation can be limited.
3. **Water quality:** Whilst it is recognised that raw water quality can inhibit abstraction from some rivers not all member companies have built these relationships into their simulation models. However, some companies do use their simulation models to understand the impact of these constraints on operations and potentially on source yields. We have also not used the simulation models to look at potential blending ratios of treated water quality though this would be advantageous.
4. **Deployable output:** Most companies use their simulation models to determine the conjunctive use of their systems for their own company; not for the region. Producing DO values for the regional is a critical output of the WRSE simulation model.
5. **Input data sequences:** Typically, all member companies have generated their own input sequences for their simulation models. These input sequences are typically generated outside the model and imported although some sequences are generated in the model.
6. **Operational and drought triggers:** Each simulation model that has been generated by the company will contain a set of operational and / or drought trigger levels which have been optimised for their systems.

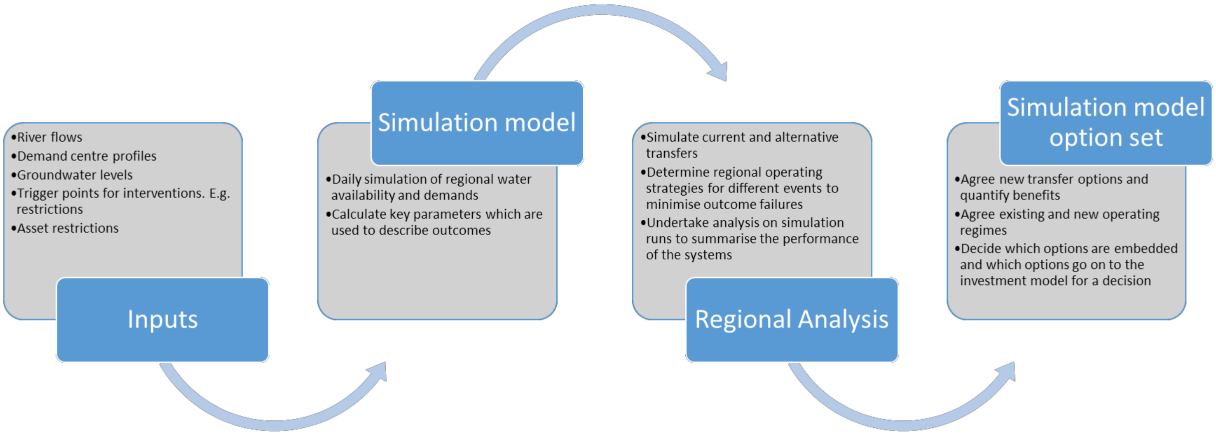
In addition to the points above it should be noted that a key purpose of the simulation model is to provide information on the current configuration and operation of the water assets, in their broadest definition, which includes other sectors' assets and operations. This is so the simulation model can be used to help determine the performance of regional water sources during different defined events which could impact on the amount of water that can be supplied to customers. Therefore, it is important that the simulation model is flexible and can take account of the above parameters changing. The defined events include:

1) Different climatic events (drought, flood);
2) Different demands for water (leakage, water use) due to temperature fluctuations;
3) Impact of third parties taking their full entitlements during extreme events; and
4) Loss of assets to treat and pump water to the customers of the region (outage, flooding, power outages, third party events such as pollution).

The current configuration of the system and its operation influences the ability to meet the demand for water in the South East. The WRSE wish to use a regional simulation model to analyse the:

5) performance of the current configuration of the system;
6) performance of the current configuration of the system but using a different mode of operation;
7) performance of the current configuration of the system but with enhanced capacities of existing transfers;
8) performance of the system with additional transfers to the current configuration of the system in the South East of England.

The results of this work could identify new physical infrastructure and new modes of operating the system that will improve the overall resilience of the region. This approach is set out in the diagram below.



Further details on how the simulation model is intended to be used are set out in Appendices A to C. These are included to allow a greater understanding of how the results from the work will be used and what areas are intended for exploration.

The timescales by which this work has to be completed by are:

1) Recommendation for the modelling approach by August 2019;
2) Regional model(s) calibrated, tested and signed off by February 2020;
3) Primary runs and analysis completed by 31 March 2020;
4) Secondary runs and analysis completed by May 2020;
5) All outputs signed off and written up by July 2020.

This scope of work covers bullet point 1 above, the review and recommendation of the optimal modelling pathway only.

5. Invitation

Please send your bid for this work by midnight on the 28th June to: Meyrick.Gough@wrse.org.uk

Your submissions should include:

1) a description of the proposed work;
2) the project team and CVs;
3) the cost for the proposed work;
4) dates for interviewing the WRSE members;
5) a programme of work including dates for deliverables; and
6) a quality assurance plan

The final report to WRSE must include:

- The recommended pathway and the reasons for its selection;
- A considered view of a forward work plan to execute the recommended pathway, given the timescales that need to be achieved, with indicative costs; and
- The risks and potential mitigation measures required to develop the recommended pathway within the PR24 timeframe.

Appendix A: Purpose and uses of the simulation model

The purpose of the simulation is to understand the resilience of the current asset base and the environment to a range of climatic events. The model would define this through the simulation of daily input date and the consequential performance of the system. The key aspect of the model is to simulate long daily time series sequences of the system, it is not the intention that this model simulates all of the catchment processes explicitly. The team should therefore outline how it proposes to simplify the various complex catchment processes in order to provide sufficient confidence that it is picking up the big challenges on water availability.

The simulation model should be based on the strategic configuration of: other sectors operation in catchments (where relevant); the current water supply systems and key discharges back into the rivers (particularly if they are linked to the operation of the water supply system).

The model will be used to simulate the catchments and regional supply systems to identify the current conjunctive use benefits of operating the system in its current and future configurations. In particular whether the mode of operation could be optimised to improve resilience across the region.

This analysis should be undertaken across a range of historic and stochastically generated climatic events in order to undertake a vulnerability analysis which covers:

1) the availability of raw water to abstract (drought, water quality) based on current and future abstractions and discharges back to the catchments;
2) increase the demand for water (leakage, water use) due to temperature fluctuations; or
3) the availability of assets to treat and pump water to the customers of the region (outage, flooding).

The outputs of this work would be to identify which zones are vulnerable to which climatic extremes and in particular which duration droughts.

Having undertaken this analysis, the model would then be used to determine how the resilience of the existing asset system could be improved through greater connectivity and or improved reliability of assets by enhancing the current system. This approach would then identify those key schemes which could balance out the risk of failure across all of the zones. The enhanced schemes should be noted and introduced as options to the investment model.

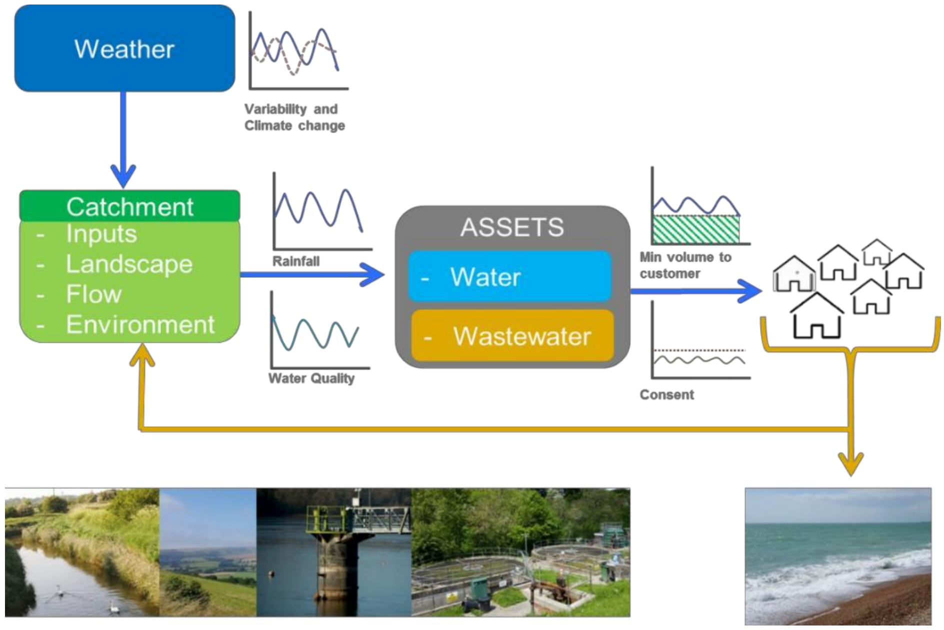
Other uses of the model will be to be used as an operational drought management model capable of demonstrating the likelihood of system failure over the next 12 months based on the simulation of current operational asset base, potential planned outage events and a range of likely climatic events, given the antecedent conditions to date.

The model will also be used to simulate the enhancement of the regional supply system by the assets identified through the investment model.

The model should be developed over a series of stages. Progression to the next stage is based on sign off of the stage, which will be subject to peer review. The proposed bid should make it clear where these break points are and where the team is proposing to seek technical sign off of the model.

Appendix B: Input data anticipated to build the regional model

In order to develop a regional model, it is anticipated that data sets across the following key asset bases would be required:



The reference to the wastewater assets in this modelling context is to highlight that some wastewater discharges are key to supporting flows in rivers which are then subsequently abstracted. These should be scoped and agreed at an early stage of the process. A cursory list of the information required by the project would contain the following data sets, which would have to be collected either from the water companies, the Environment Agency or third-party sources.

1. Catchment rainfall runoff models in order to generate new time series of river flows;
2. Recharge models to generate appropriate groundwater levels, where appropriate;
3. Strategic trunk main maps showing the water supply systems for each of the companies or print outs of existing simulation models;
4. Other abstractors and discharges including an analysis of need and materiality of other abstractions to determine whether to model their uptake. This could lead to the development of potential new schemes including licence trading.
5. Raw water quality in the rivers and groundwater for keys parameters, where available;
6. Input climate data sets would include spatially coherent droughts of different magnitudes and durations (these may require further work to ensure they are coherent with national data sets);
7. Drought triggers for key catchments or key observational hydrometric stations (groundwater levels; river gauging stations, etc)
8. Distribution input data, broken down into WRZs and demand centres from existing models, where appropriate, in order to determine the effect of temperature on the demand for water;
9. Leakage data at a DMA level to understand the impact of temperature on leakage at a water resource zone level;
10. Review the groundwater deployable output assessments undertaken by the companies to understand whether the groundwater modelling used within the companies can be used to generate appropriate input sequences into the regional simulation model;
11. Imports/ exports to the region
12. Standardise cost development method for third parties to provide costs for options to be assessed by any WRSE partner
13. Ensure 3rd parties also using equivalent/ minimum timeframes and drought analysis
14. An agreed level of service for individual companies and the region, which will have to be defined by the Programme Management Board.
15. Other abstractor drought restriction i.e. Section 57 (irrigation) should be concurrent with public water supply restrictions.

Appendix C: Model to simulate/ output

The following list of model outputs is not exhaustive, and the proposed bidder is encouraged to demonstrate what other factors could be displayed, but at a minimum the model should provide information on:

1. Abstraction and discharge data on a daily timestep;
2. Mixing of waters at demand centres;
3. A resilience index for the system based on its configuration, reliability, redundancy and ability to resist the modelled climatic data;
4. Surface water flows both natural and residual
5. An environmental index
6. Planned outages at source levels, noting that for some smaller sources this could represent an amalgamation of sources
7. Demonstrate the coincidence of some events e.g. dry winter and hot summers;
8. Performance of the system through a series of system performance metrics which might include, but an analysis of the time series data against certain thresholds;
9. Resilience of some of the systems to different duration droughts;
10. The number of lost days of pumping (both abstraction and transfers) due to water quality constraints;
11. Threshold analysis of all output time series from the model through a series of summary outputs;
12. Frequency and duration of drought permit/order use – using implementation rather than application

Once the model has been scoped and developed, it should be run at least 50 times to define the performance of the current system and how this could be optimised with the existing configuration of assets as well as the addition of new assets. This work would also include re-optimisation of control curves of key assets in the region.

Appendix D

Appendix D. Scope for Hydrological Analysis for System Simulation

Introduction

This scope of work sets out the hydrological analyses that will be required to support the development of the system simulation model for WRSE.

Objectives

This package of support will need to deliver the following output, which will be incorporated into the WRSE system simulation model.

1. Derivation of lumped parameter rainfall/runoff models for the Thames basin (River Thames and River Lea)
2. Development of algorithms that will allow the adjustment of de-naturalised flows to reflect changes in wastewater discharges and licence trades for the following catchment assessment points:
    a. The River Thames at Teddington and Days Weir
    b. The River Lea at Fieldes Weir
    c. The River Chess (assessment point to be determined)
    d. The River Rother at Hardham
    e. The River Medway at the Burham intake
    f. The River Itchen at Highbridge and Allbrook
    g. The River Test at Broadlands
    h. The River Stour (assessment point to be determined)
    i. The River Wey (assessment point to be determined)
    j. The River Medina (assessment point to be determined)
3. Generating flows at the relevant assessment points for the new lumped parameter rainfall/runoff model for the River Thames using the WRSE stochastic rainfall and PET data set.
4. Development of algorithms based on flow-duration curves (FDC) that will allow the impact of reductions in groundwater abstraction to be modelled (particularly where these are related to sustainability reductions), for the same catchment assessment points as detailed above.
5. Development of algorithms that will allow the simulation of Deployable Output based on rest groundwater level input timeseries, using existing relationships for scaling of groundwater levels into peak, average and (where available) minimum period DO.
6. Develop algorithms that will allow simplistic representation of effective available abstraction for hydrogeologically constrained groundwater sources.

Specifications

The key requirements, performance criteria and assumptions for each of the objectives are set out in Table 1 below.

Objective	Requirement	Performance Criteria	Assumptions
1.River Thames and River Lea lumped parameter models	Flows need to be generated based on a number of sub-catchments (circa 11), adequate to match the recession and spate behaviour in the WARMs model.	The generated hydrology needs to be able to support the system simulator so it can match the Deployable Output of the key 20th century droughts (1921 and 1934) for the London WRZ to within +/-50Ml/d	Model parameters for the existing lumped catchment models at Fieldes Weir, Days Weir and Teddington Weir will be provided. Historic flow timeseries from WARMs will be provided.
2.De-naturalisation algorithms	Evidence based analyses of the tradeable licence and WWTW catchments that provides the system simulation team with the inputs required to simulate flow variation due to changes in demand and licence trading	HoF constraints on potentially tradeable licences and agreed proportions of demand returns for the catchment assessment points.	Data on returns will need to be gathered from water companies. HoF constraints will need to be gathered from EA licence databases, limited to significant licences.
3. Flows for the new River Thames lumped parameter model	Generate daily flows for circa 20,000 years of data based on WRSE stochastic data set	Validation checks on FDCs for the stochastic data set versus the historic data set to confirm no bias has been introduced.	Rainfall and PET data provided in a compatible format from WRSE.
4.FDC based benefits from sustainability reductions	Evidence based assessments of the relative impact that reductions in catchment groundwater abstractions have on the flows at the relevant modelled points, based on Flow-Duration Curve Q percentiles (see Figure 1).	Values will be simple ratios, with an average of 1 (or less if there is evidence of likely increased groundwater loss from the catchment). Need to ensure that the evaluation is evidence based with appropriate audit trails	Information will need to be gathered from sustainability reduction investigations from water companies.
5.Groundwater DO algorithms: annual constraints	Factors, set by WRZ, that will allow input GWL timeseries to be translated into ADO, PDO and (if required) MDO values that will vary by year depending on the GWL timeseries.	Sets limits on abstraction for hydrogeologically constrained sources. It is anticipated that only two limits will be used – PDO (applied over the summer months) and non-PDO (all other months), although this will need to be consulted on. The translation will need to be taken from water companies' WRMP19 groundwater DO assessments, with audit trails demonstrating evidence and consistency with the WRMPs	Primary analysis is not required – only needs liaison with water companies to access their WRMP19 DO generation.

6.Groundwater DO: volumetric capability	Incorporate algorithms into the DO mechanism that allow for volumetric limits on abstraction. The concept is that within the absolute limits set by the PDO/non-PDO, there is a maximum amount that can reasonably be taken during the summer months (i.e. sources cannot run at PDO for 3 months) (see Figure 2).	Need to agree the approach with individual water companies. Groundwater storage models are not included in the scope – this is intended to be a simplistic representation based on past operational experience. The constraint could to be derived from past Distribution Input traces, but the final method needs to be evidence based.	Need to liaise with water companies to understand and evidence approach. Calibration is not required.

The concept behind specification number 4 is relatively straightforward, although the values assigned will need to be evidence based from ongoing NEP investigations by water companies. This is illustrated in Figure 1 below.

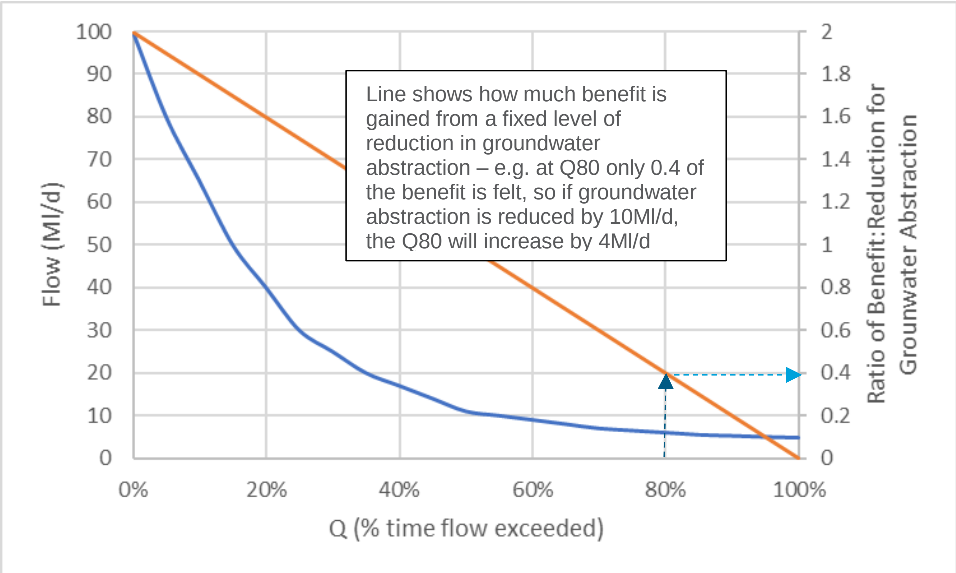


Figure 1 – Example Chart of Benefit versus Flow Percentile for Reductions in Groundwater Abstraction

The concept behind specification 6 is illustrated in Figure 2 below. Effectively this algorithm prevents excessive abstraction from groundwater when it is being analysed conjunctively with surface water storage sources. The way that the annual total abstraction allowance is calculated is open to analysis (e.g. it could be based on historic DI profiles, which indicate how much has historically been taken from groundwater sources under drought conditions and hence sets the constraints on the validity of the source DO diagrams) but will need to be evidence based.

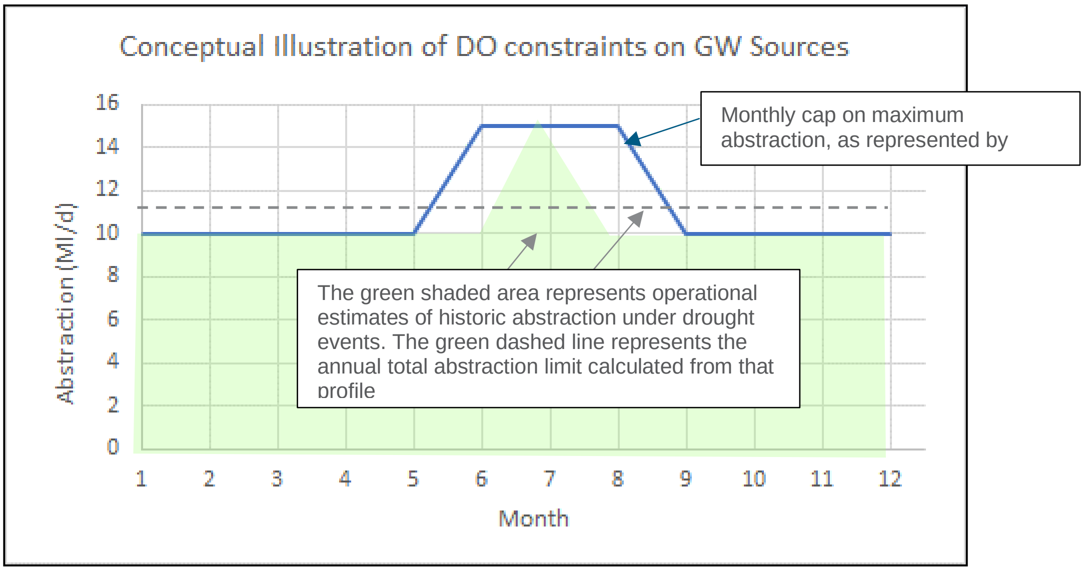


Figure 2 – Conceptual Illustration of Volumetric Constraint for Groundwater Sources

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