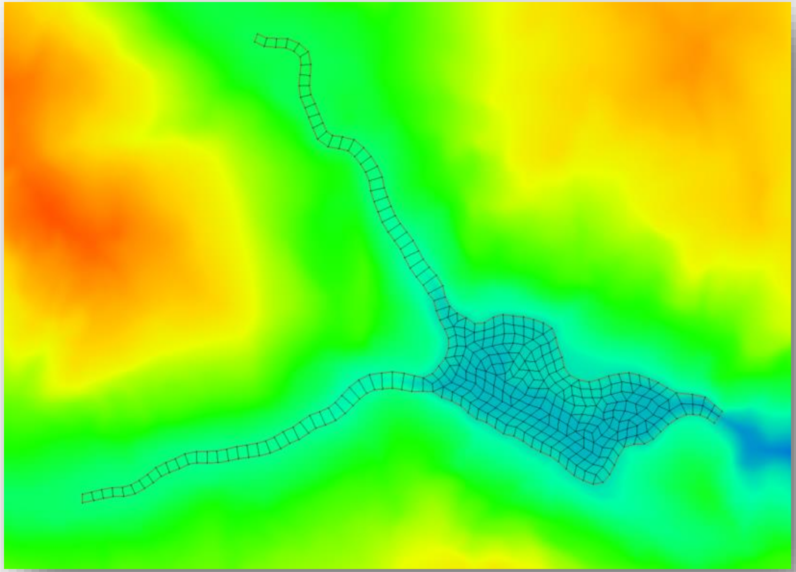
Simulation, modelling and analysis of the living water system: Improving our beneficial return on investment

Modelling Symposium 2024
Christchurch - Workshop 1
12th March 2024

Workshop 1
Agenda

This afternoon (very roughly)

- 3:00 – 3:05: Introductions and intent
- 3:05 – 3:20: The hypothetical
- 3:20 – 3:30: Peer review: sediment
- 3:30 – 4:00: Peer review: dissolved oxygen
- 4:00 – 4:20: Peer review: chlorophyll a
- 4:20 – onwards: Key messages and wrap



TUFLOW

BMT

Introductions

Workshop 1
Introductions

Michael Barry

- Based in Brisbane, Australia
- Undergrad degrees and PhD from the University of Western Australia
- 28 years industry experience
    - Environmental hydrodynamic and water quality modelling
    - Systems analysis
- 5 years at TUFLOW

Workshop 1
Introductions

Mitchell Smith

- Based in Brisbane, Australia
- Undergrad degrees from the University of QLD and University of Southern QLD
- 18 years consulting experience
  - Coastal hazards
  - Flooding
  - Environmental modelling
- 9 years at TUFLOW

Workshop intent

Workshop 1
Intent

Workshop

- Use a hypothetical environmental system and model to explore ways to improve beneficial return on modelling investment
- Support better management of the living water system
  - Use of model predictions beyond traditional timeseries
  - Ways and tools to engage more broadly and effectively
- Explore use of models for understanding (not just compliance)
- Ways to save time and money in the calibration process
- Materials for group use on tables

The hypothetical

Workshop 1
The hypothetical

The premise

- A (made up) New Zealand water supply reservoir has a recurrent January phytoplankton bloom problem, with dissolved oxygen issues at depth
- A 3D hydrodynamic and water quality model has been built and ‘calibrated’ to assist in managing/remediating the reservoir and/or catchment from which it drains
- Michael and I are the modelling Project Managers
- You are all peer reviewers of our company’s model, acting on behalf of the customer
- Goal is to approve the model for scenarios and therefore management assessment
  - Is the model “right” or “fit for purpose”?

Workshop 1
The hypothetical

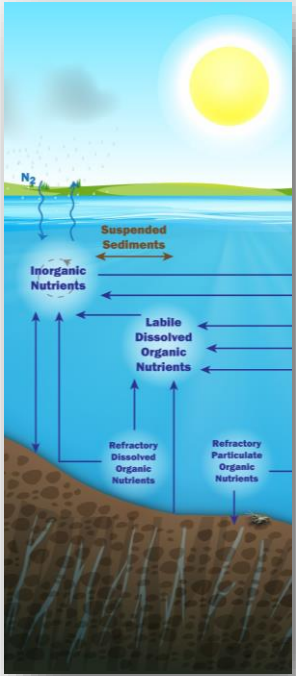
The premise

- Michael and I are
  - Out of time
  - Out of money
- You are all peer reviewers of our model, acting on behalf of the customer
  - Peer review has been left to the 11th hour
  - No prior involvement in the modelling
  - You (rightfully!) have high standards

Workshop 1
The hypothetical

The system

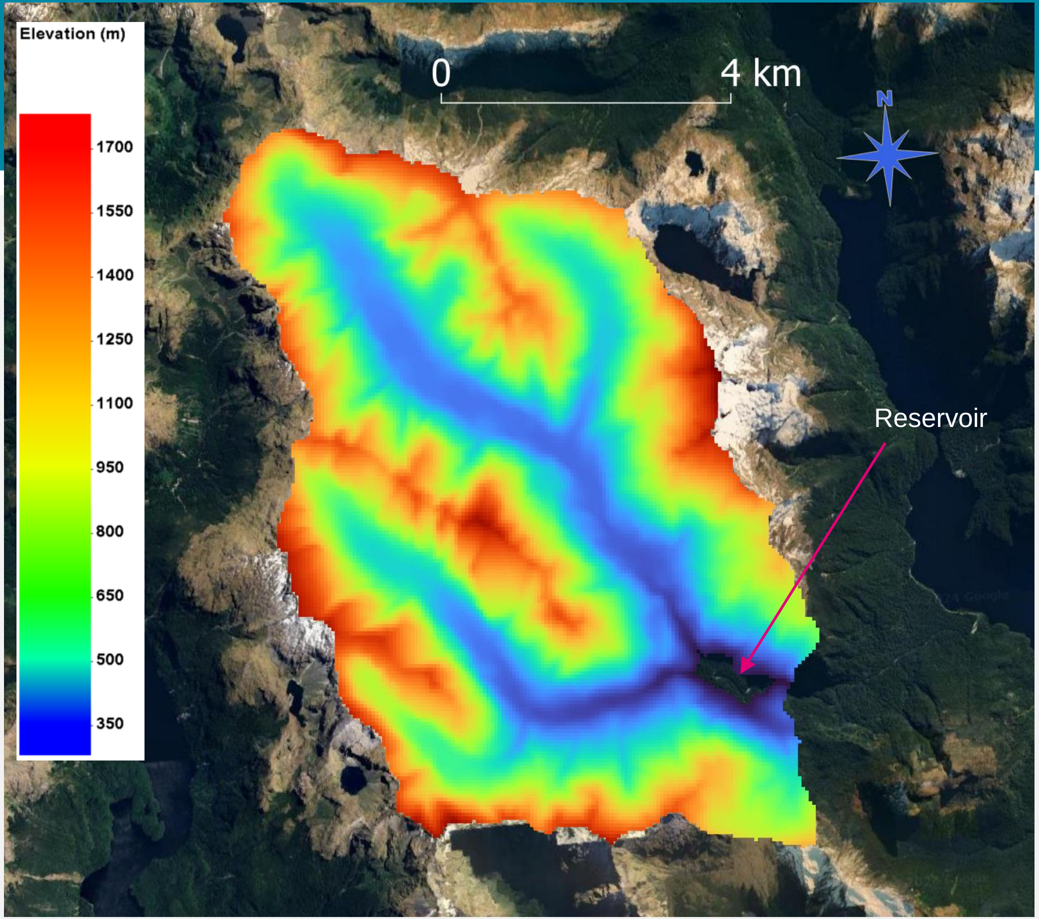
- Catchment
  - 5473 hectares
  - 2534, 2397 and 542 ha forest, agriculture and urban
  - ~700mm annual rainfall
- Reservoir
  - 200 hectare surface area
  - Maximum depth ~35m
  - One offtake and two legacy point source discharges



Workshop 1
The hypothetical

The system

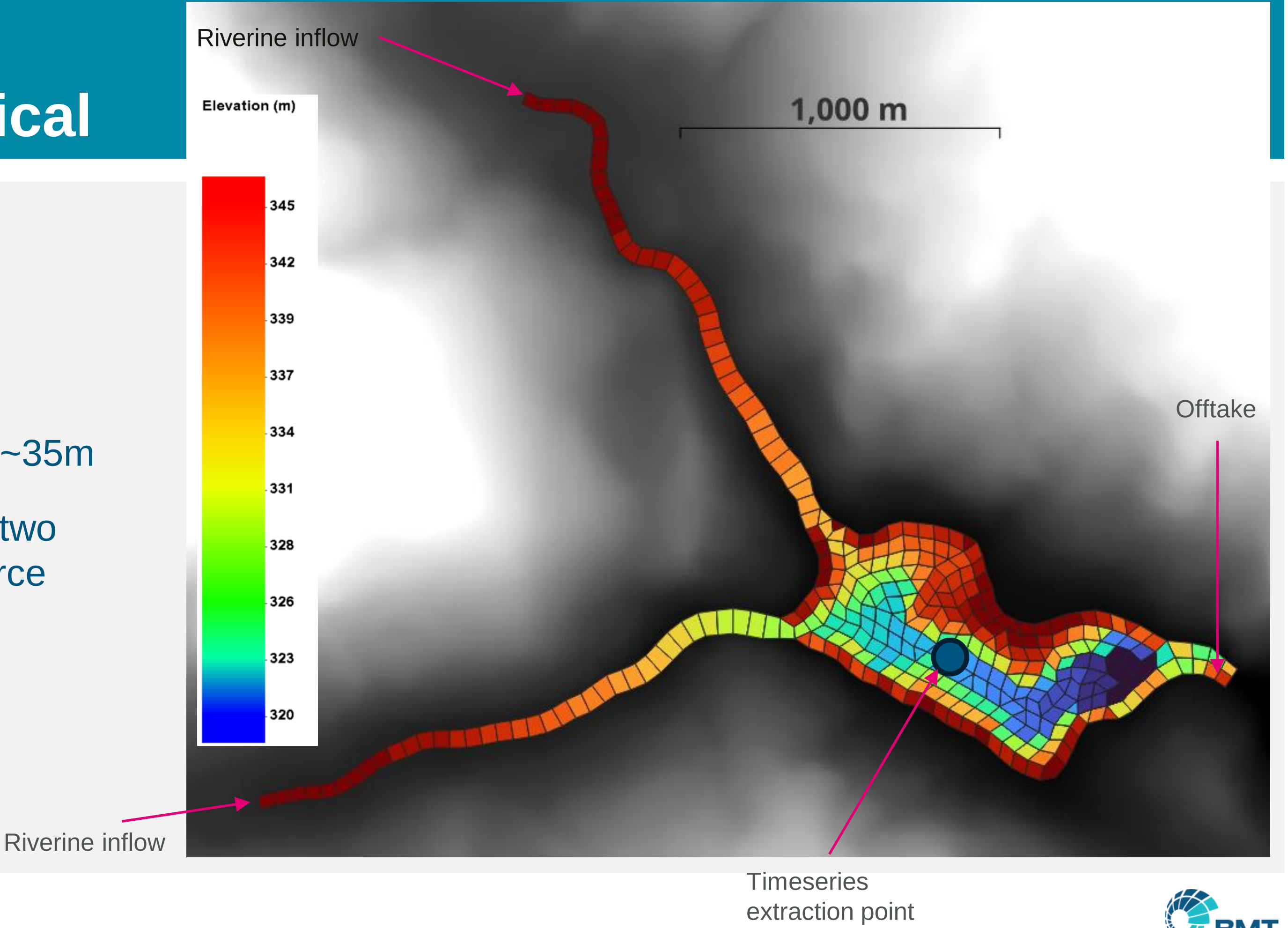
- Catchment
  - 5473 hectares total
  - 2534 ha forest,
  - 2397 ha agriculture
  - 542 ha urban
  - ~700mm annual rainfall



Workshop 1
The hypothetical

The system

- Reservoir
  - 200 hectares
  - Maximum depth ~35m
  - One offtake and two legacy point source discharges



Workshop 1
The hypothetical

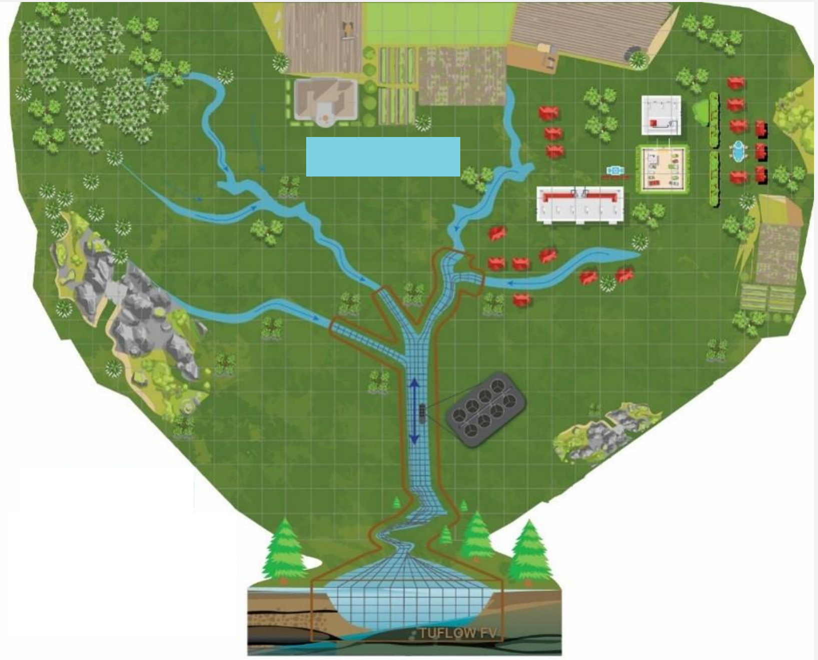
The system

- Known issues
  - Summer (January) algal blooms
  - Low dissolved oxygen at depth
  - Sedimentation from catchments
  - Catchment is very poor in organics
  - Sludge exists at the bottom of the reservoir
  - Urbanisation has made green blooms much worse
  - Nitrates are high at the downstream water treatment plant

Workshop 1
The hypothetical

The system

- Build a system model to assist management



Workshop 1
The hypothetical

The modelling system

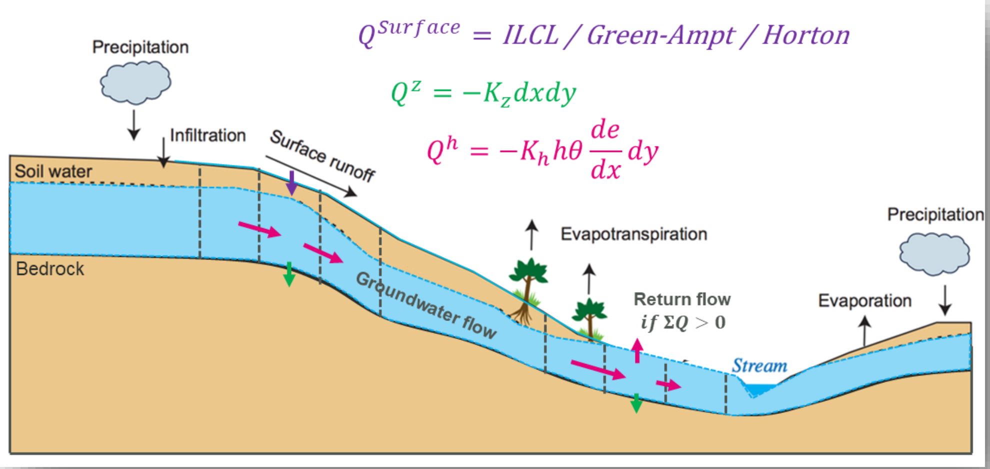
- 1 month simulation (usually would do more!)
- High spatial and temporal resolution throughout
- Seamlessly integrated catchment and receiving water quality model
  - TUFLOW HPC
  - TUFLOW FV

TUFLOW Catch

Workshop 1
The hypothetical

The model

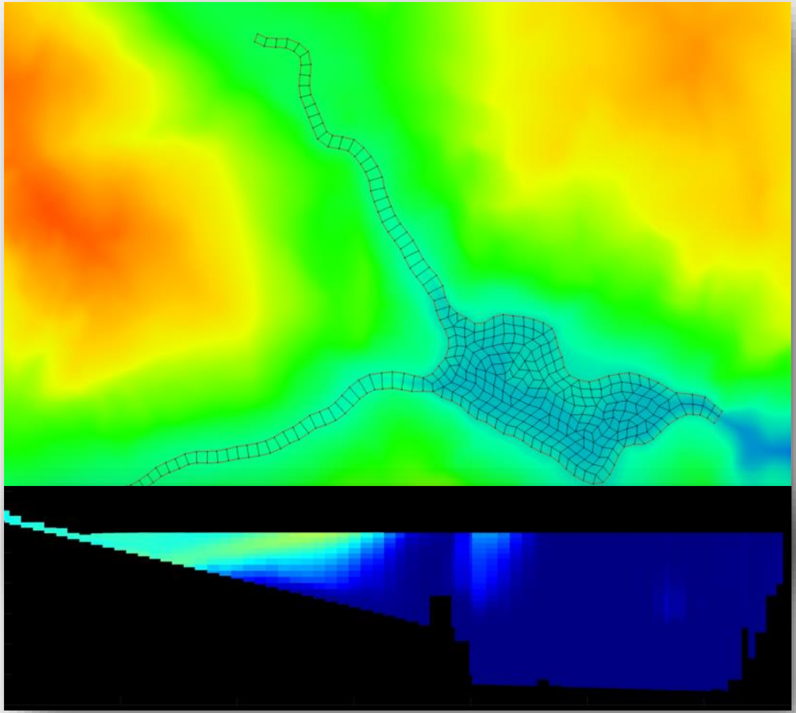
- Catchment
  - Fixed grid, direct rainfall, solves equations of motion to predict surface and subsurface hydrology on a 50m cell
  - Pollutant accumulation and washoff model (user parameterised) also on 50m cell
  - Automatic linkage of simulated flows and loads of speciated constituents to receiving model



Workshop 1
The hypothetical

The model

- Receiving
  - Flexible mesh
  - 3D HD (water surface, velocity, temperature, suspended sediment), multiple vertical layers
  - 3D water quality (oxygen, inorganic and organic nutrients, one phytoplankton)
  - Would normally have higher spatial resolution in inflows – suitable for demonstration
  - ~ 25 x 3D layers at 1m vertical resolution



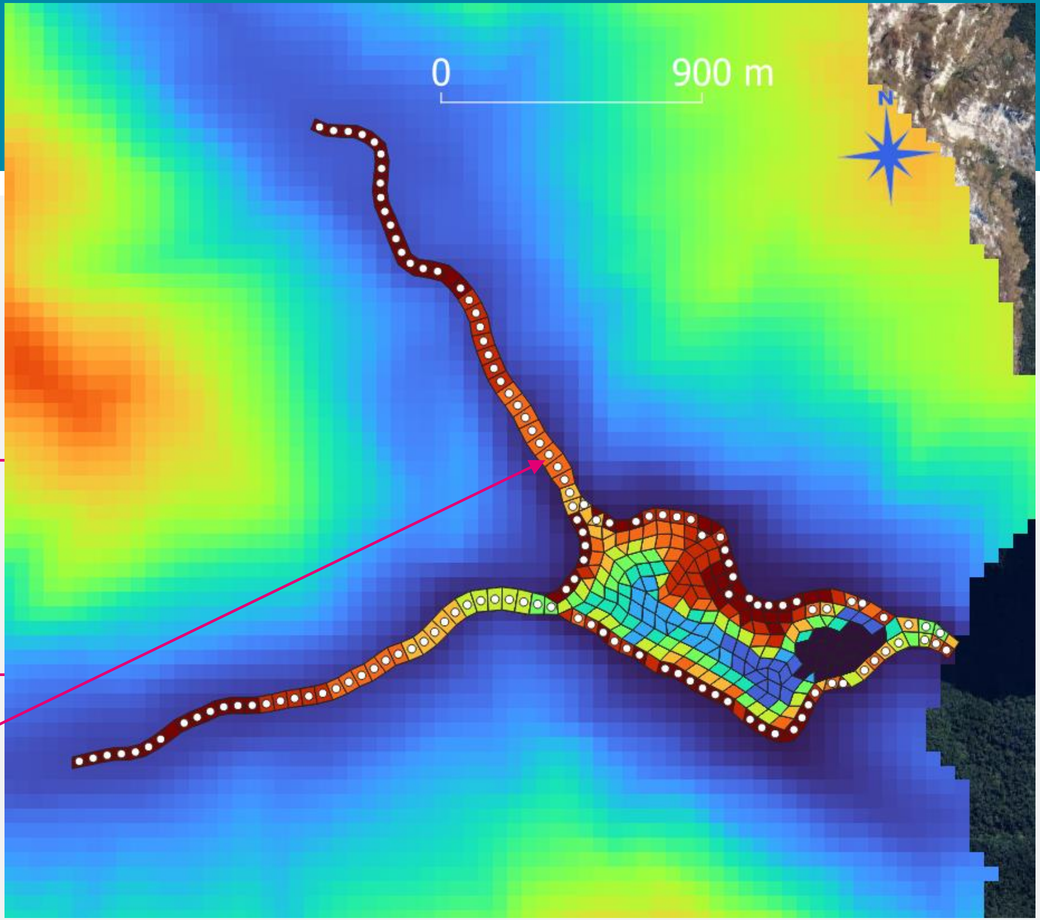
Workshop 1
The hypothetical

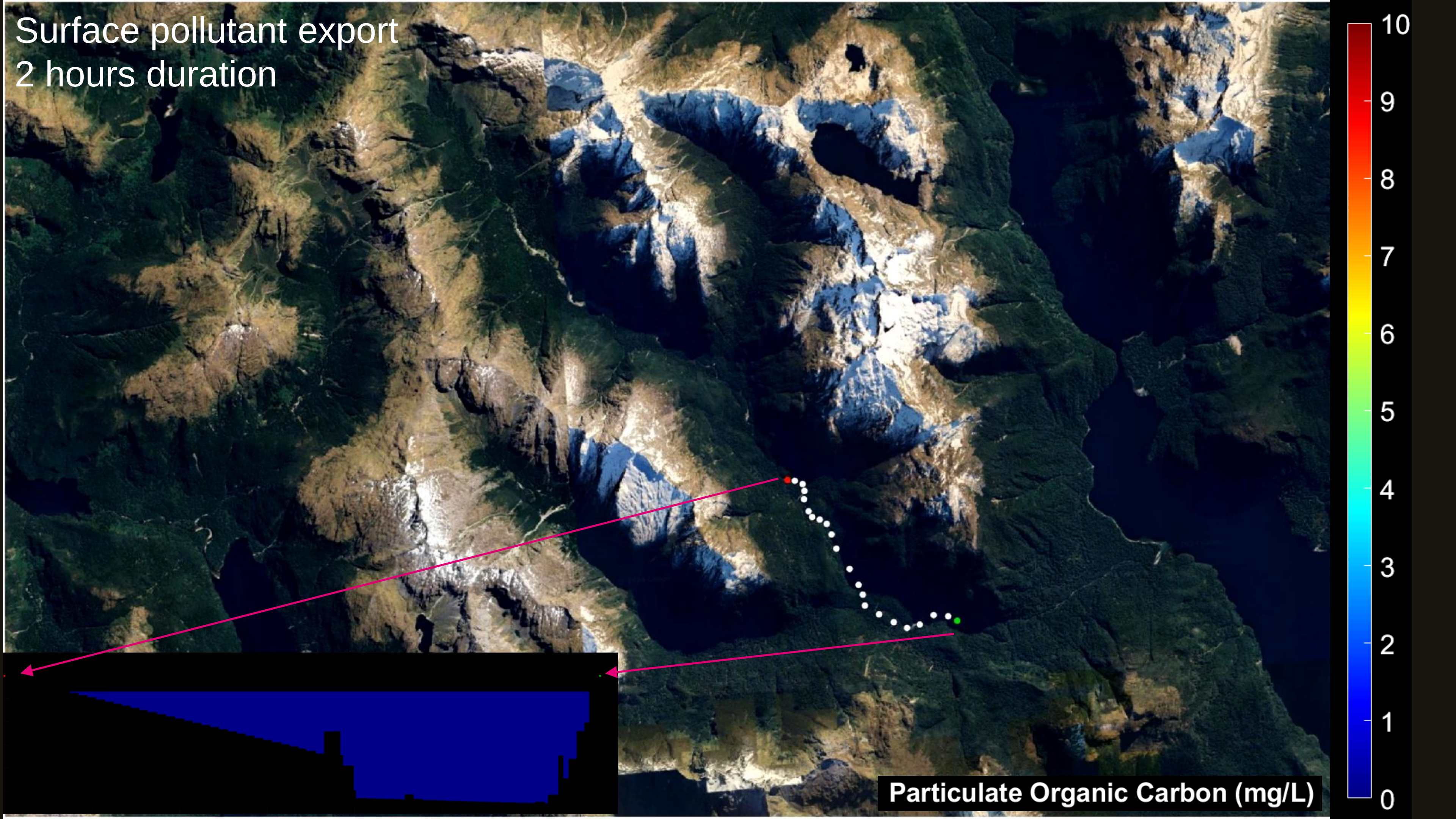
The model

TUFLOW HPC Domain

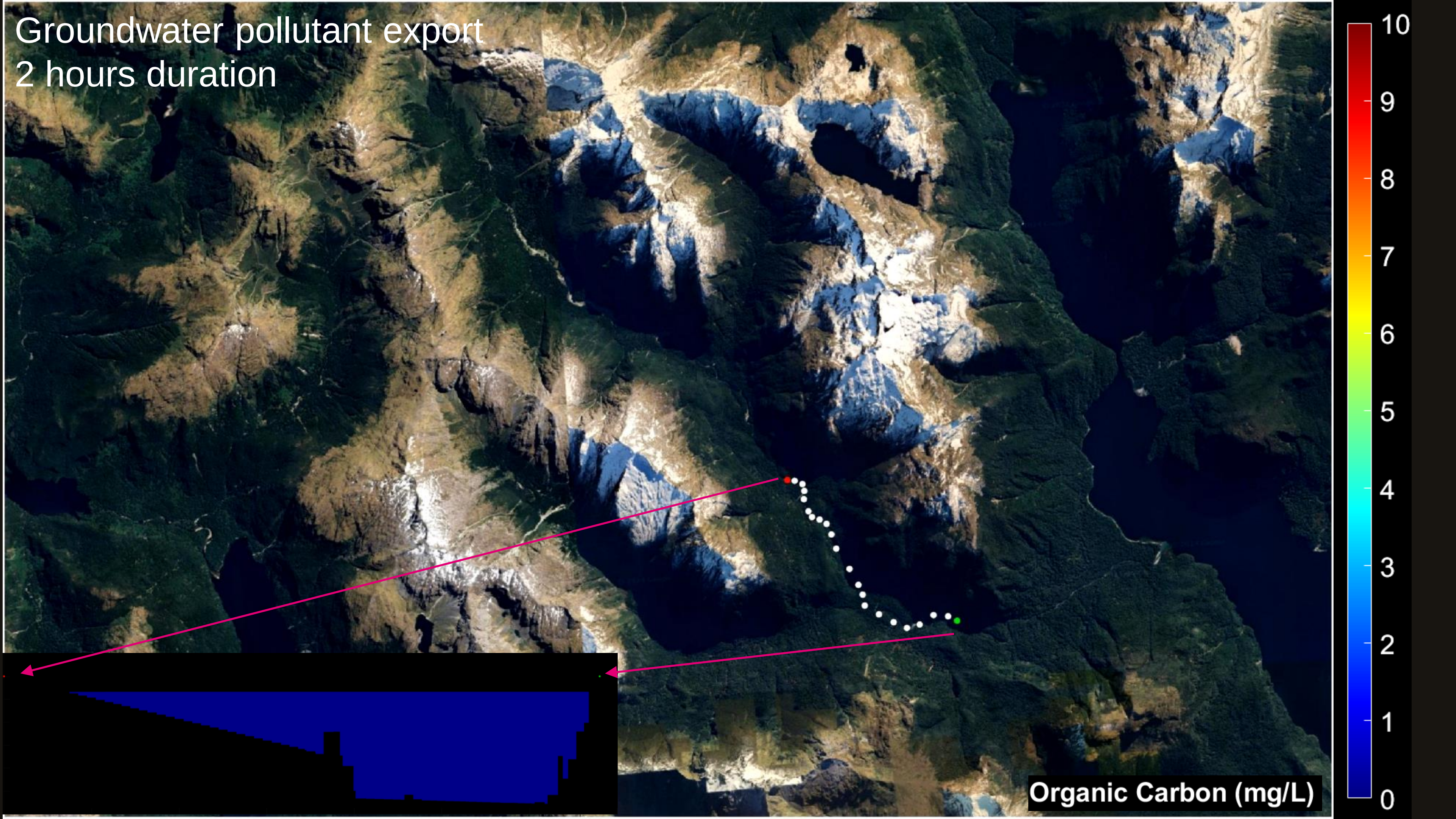
TUFLOW FV Domain

Automatically determined
connection boundary points
(white dots)

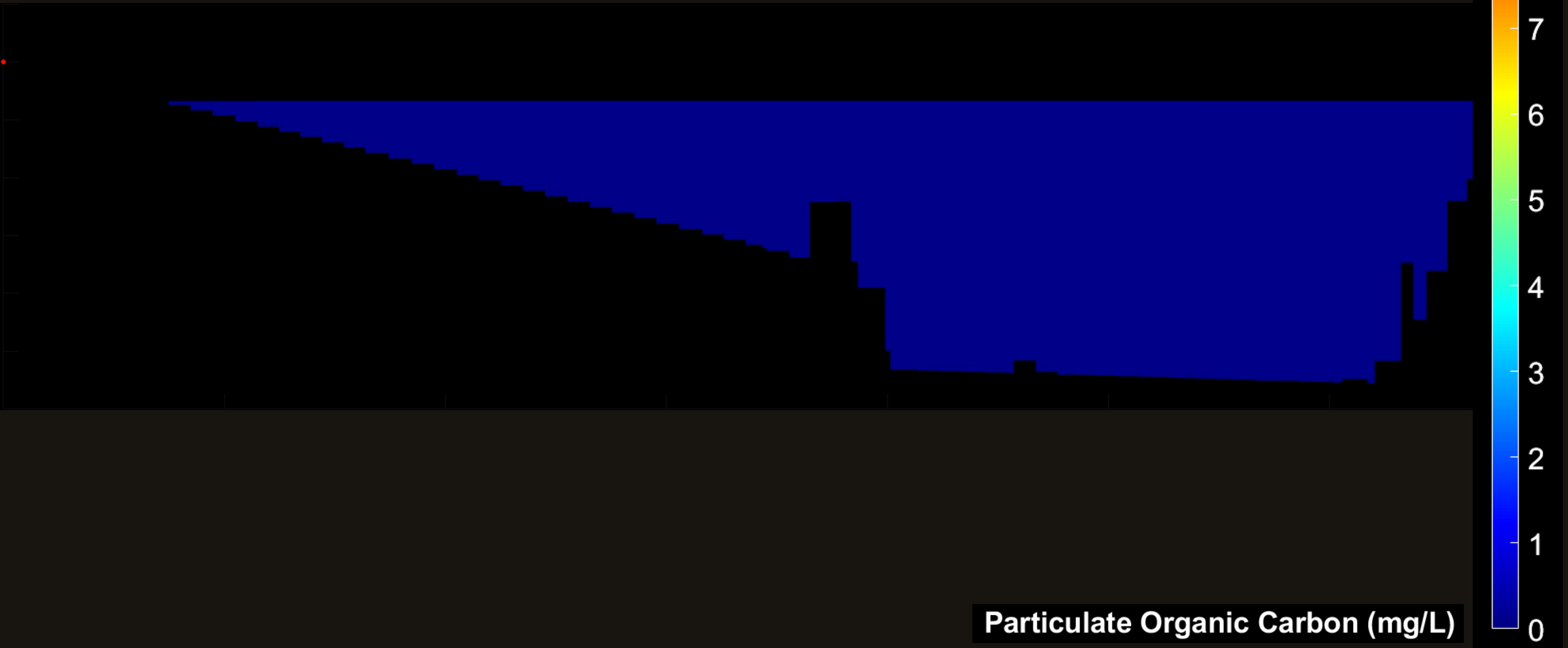




Surface pollutant export
2 hours duration
Particulate Organic Carbon (mg/L)
10
9
8
7
6
5
4
3
2
1
0


Groundwater pollutant export
2 hours duration
Organic Carbon (mg/L)
10
9
8
7
6
5
4
3
2
1
0

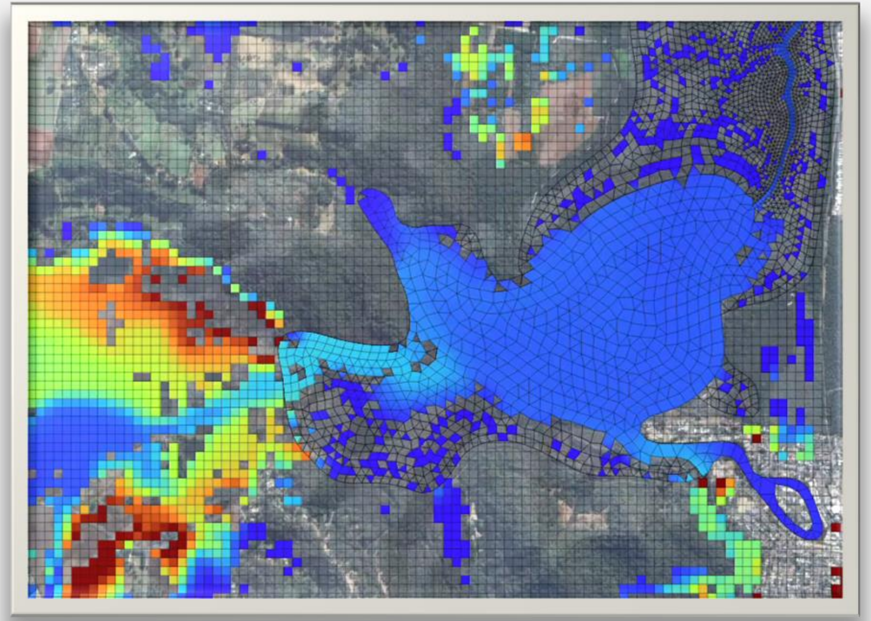
Catchment inflow
12 hours duration



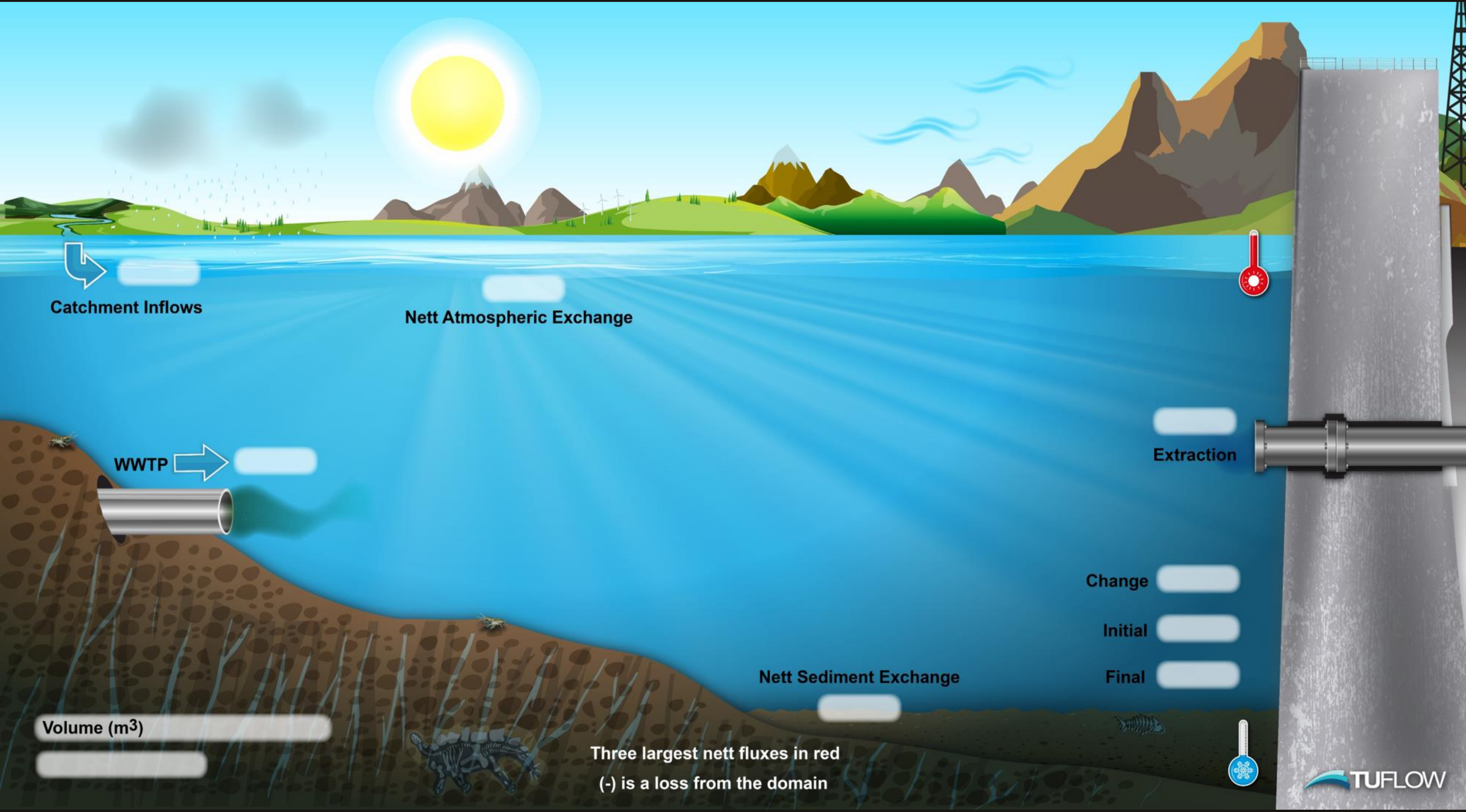
Workshop 1
The hypothetical

The model

- Could look at all constituents, but focus on
  - Volume
  - Suspended sediment
  - Dissolved oxygen
  - Phytoplankton



The hypothetical: Volume



Catchment Inflows
Nett Atmospheric Exchange
WWTP
Extraction
Change
Initial
Final
Nett Sediment Exchange
Volume (m3)
Three largest nett fluxes in red
(-) is a loss from the domain
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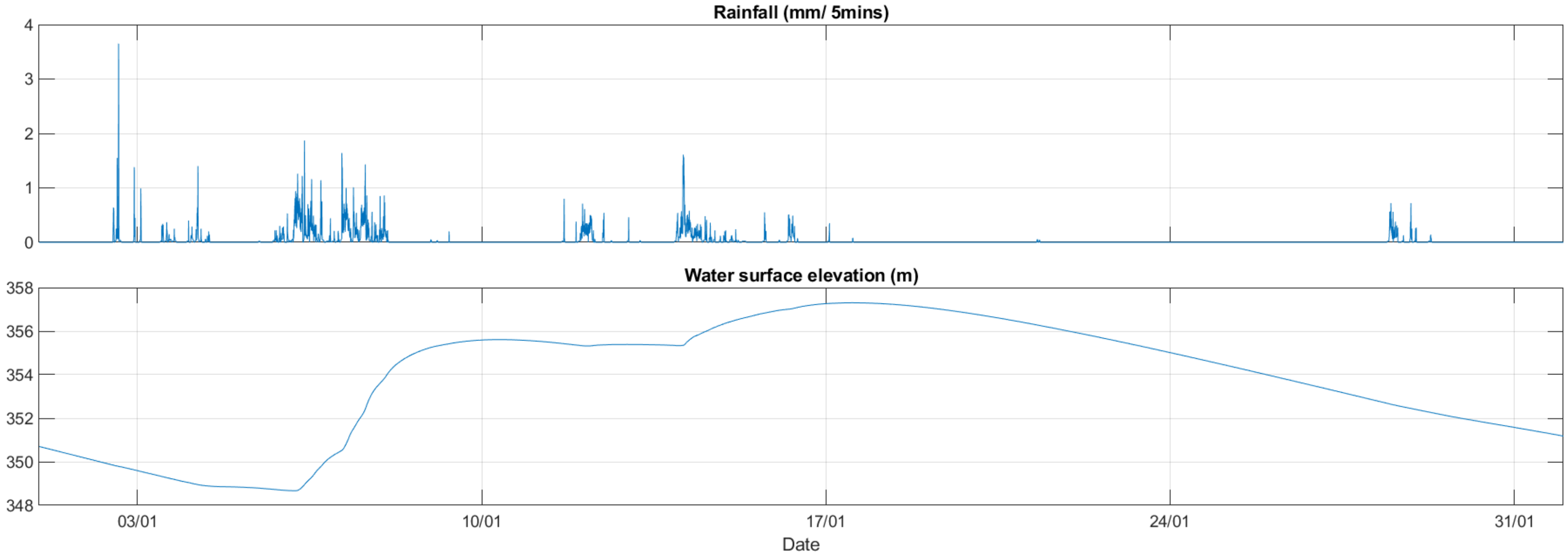
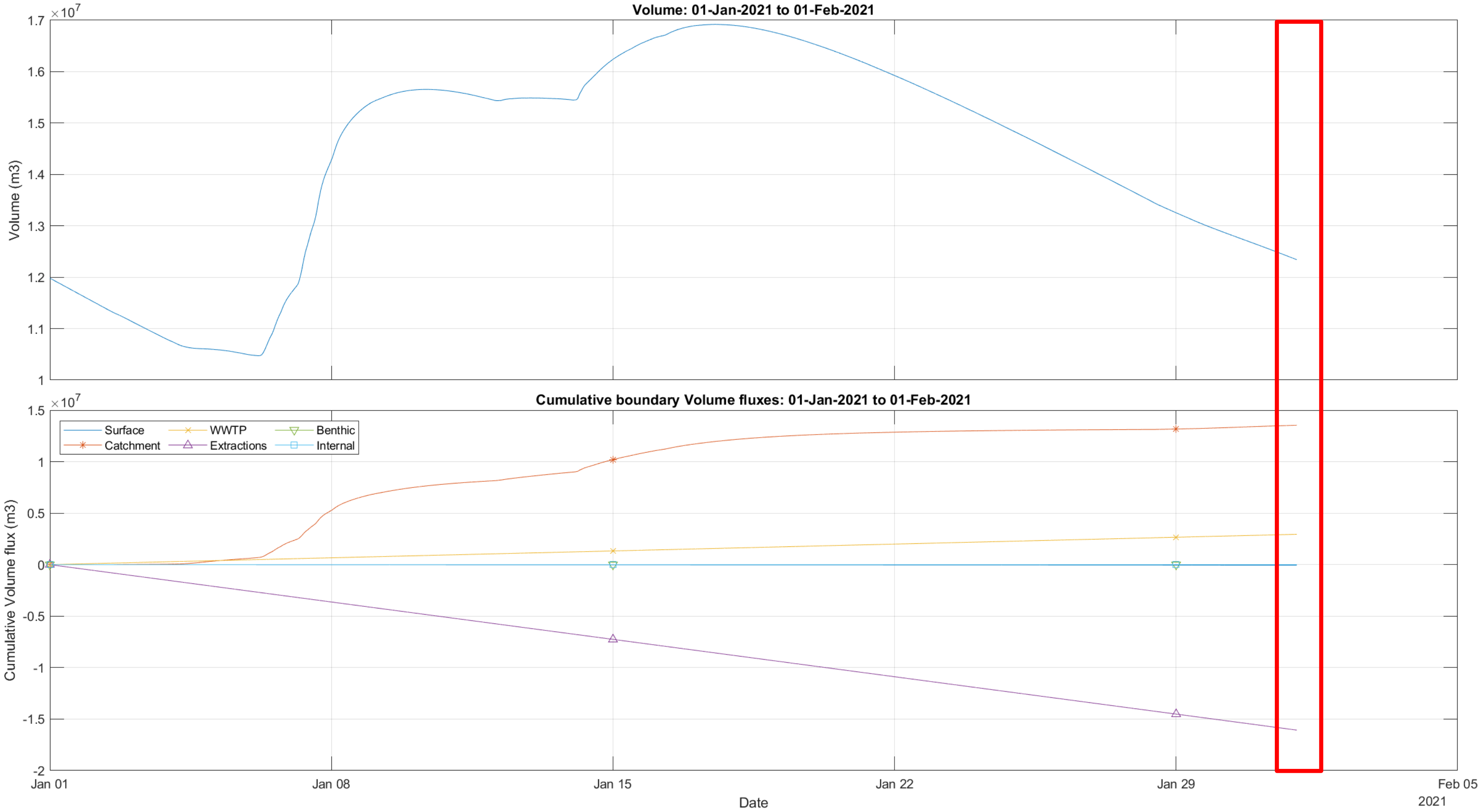
Workshop 1
The hypothetical

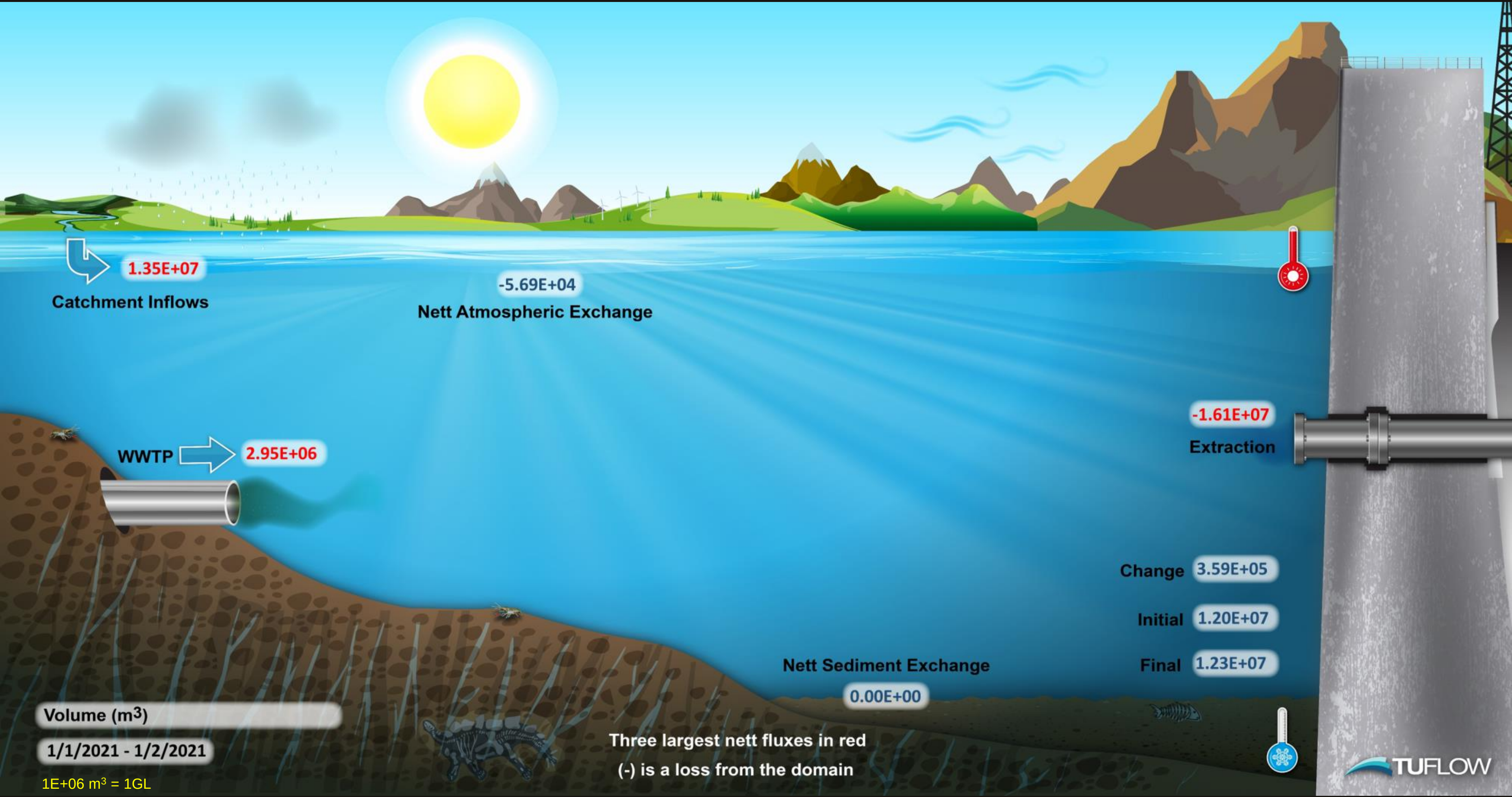
Volume

Mm/hr





Volume: 01-Jan-2021 to 01-Feb-2021
Volume (m3)
×10^7
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
Cumulative boundary Volume fluxes: 01-Jan-2021 to 01-Feb-2021
Cumulative Volume flux (m3)
×10^7
1.5
1
0.5
0
-0.5
-1
-1.5
-2
Surface
Catchment
WWTP
Extractions
Benthic
Internal
Jan 01
Jan 08
Jan 15
Jan 22
Jan 29
Feb 05
2021
Date


1.35E+07
Catchment Inflows
-5.69E+04
Nett Atmospheric Exchange
-1.61E+07
Extraction
WWTP
2.95E+06
Change 3.59E+05
Initial 1.20E+07
Final 1.23E+07
Nett Sediment Exchange
0.00E+00
Volume (m3)
1/1/2021 - 1/2/2021
1E+06 m3 = 1GL
Three largest nett fluxes in red
(-) is a loss from the domain
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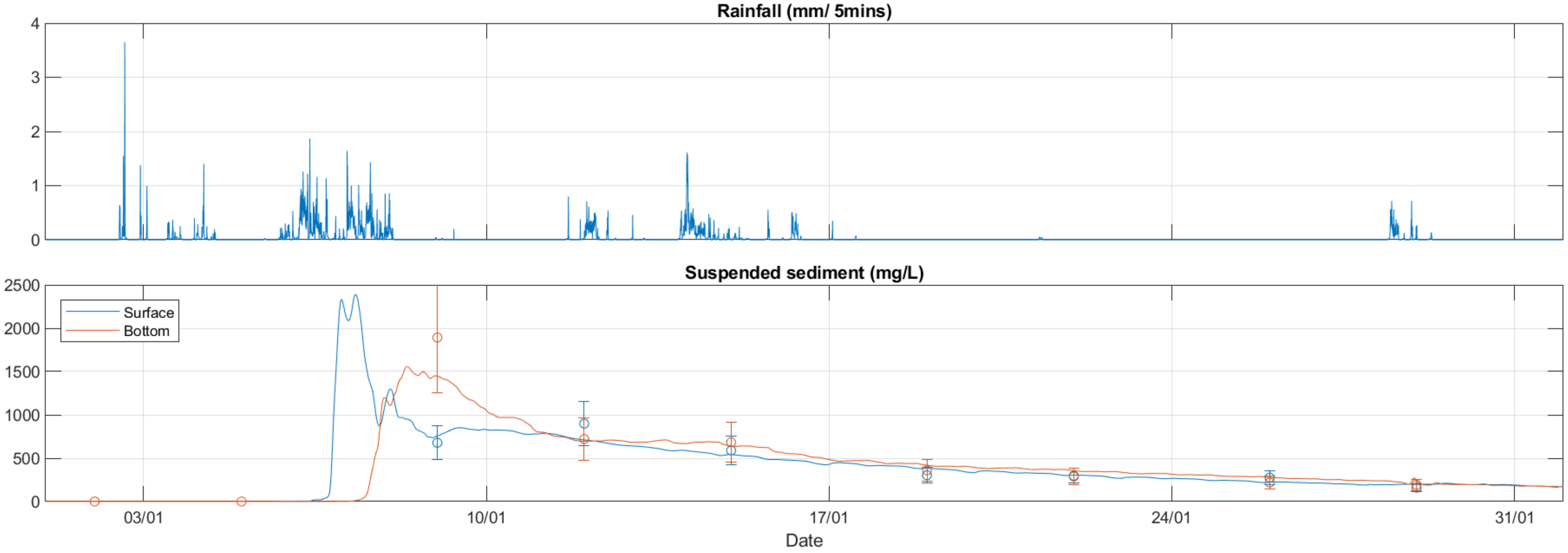
The review:
Suspended sediment

Workshop 1
The review

Sediment concentration timeseries



Workshop 1
The review

Sediment concentration stats

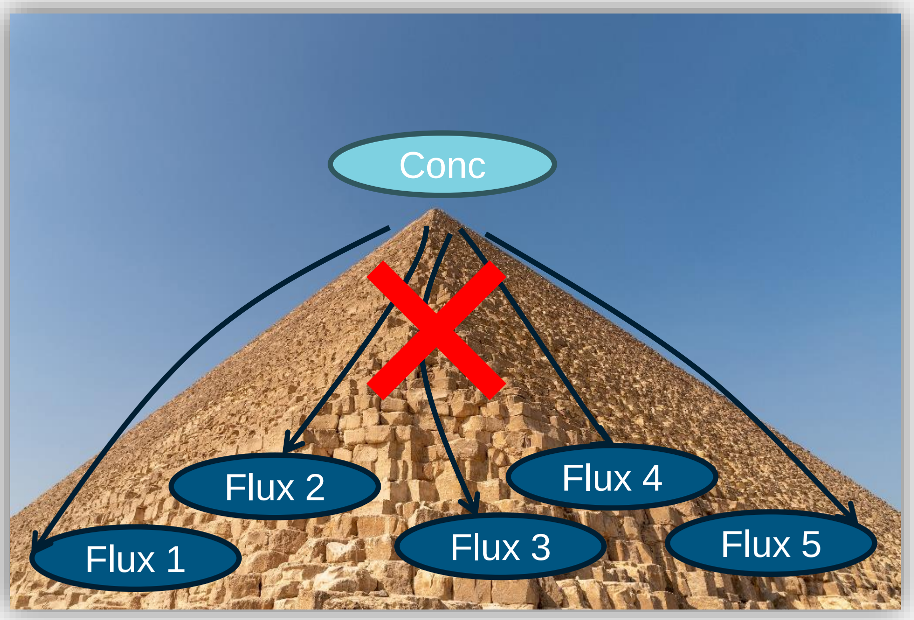
- Prediction / calibration of concentrations
- Moriasi et al. 2015 and others
  - Very good
  - Good
  - Satisfactory
  - Not satisfactory

Metric	Value
R	0.98
R2	0.96
NSE	0.92
IOA	0.98
RMSE	122
MAE	69
PBIAS	4.5

Workshop 1
The review

Sediment

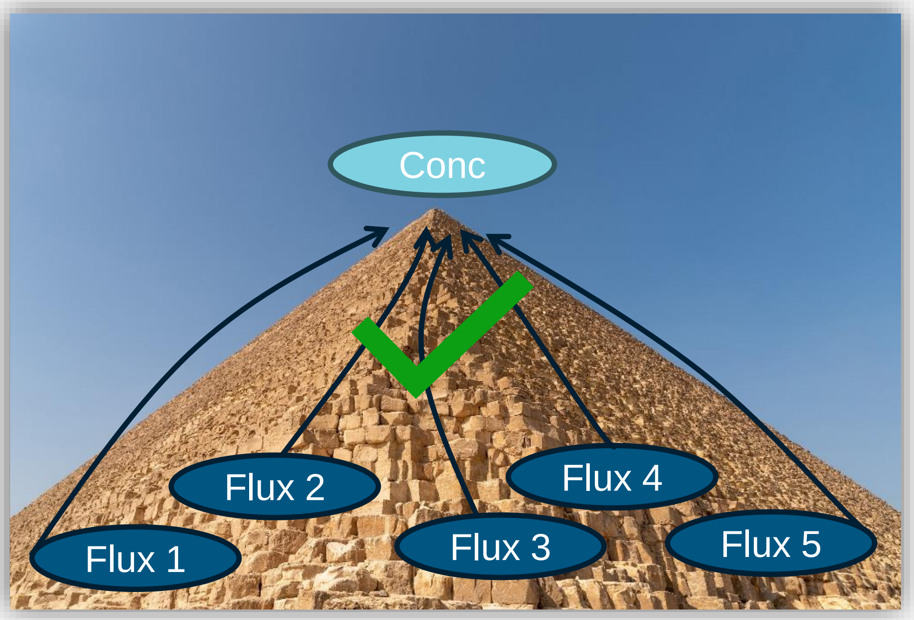
- Solutions
  - Where in the catchment do we work?
  - Integrated model
    allows us to look at fluxes
    (what we are really trying to fix)

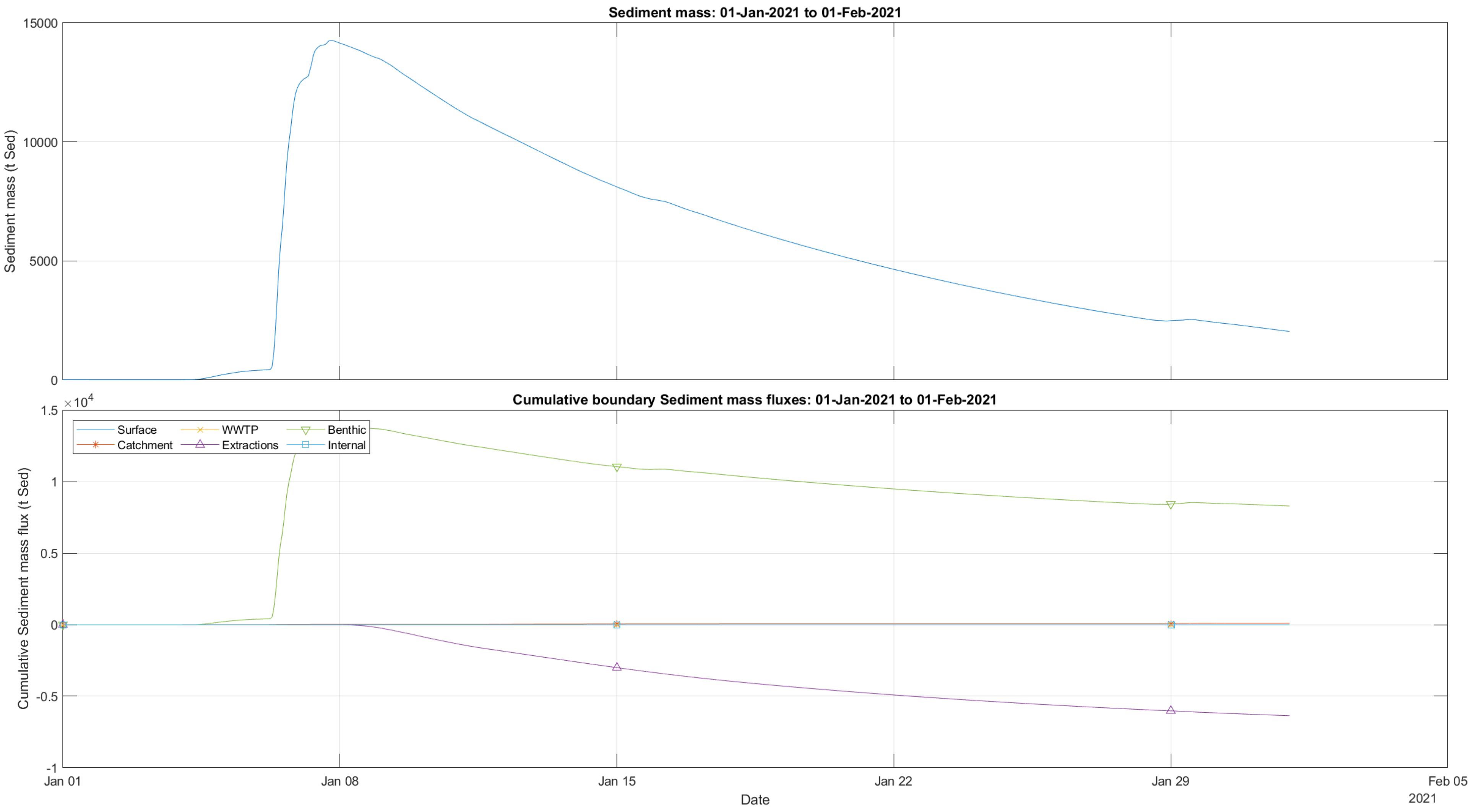


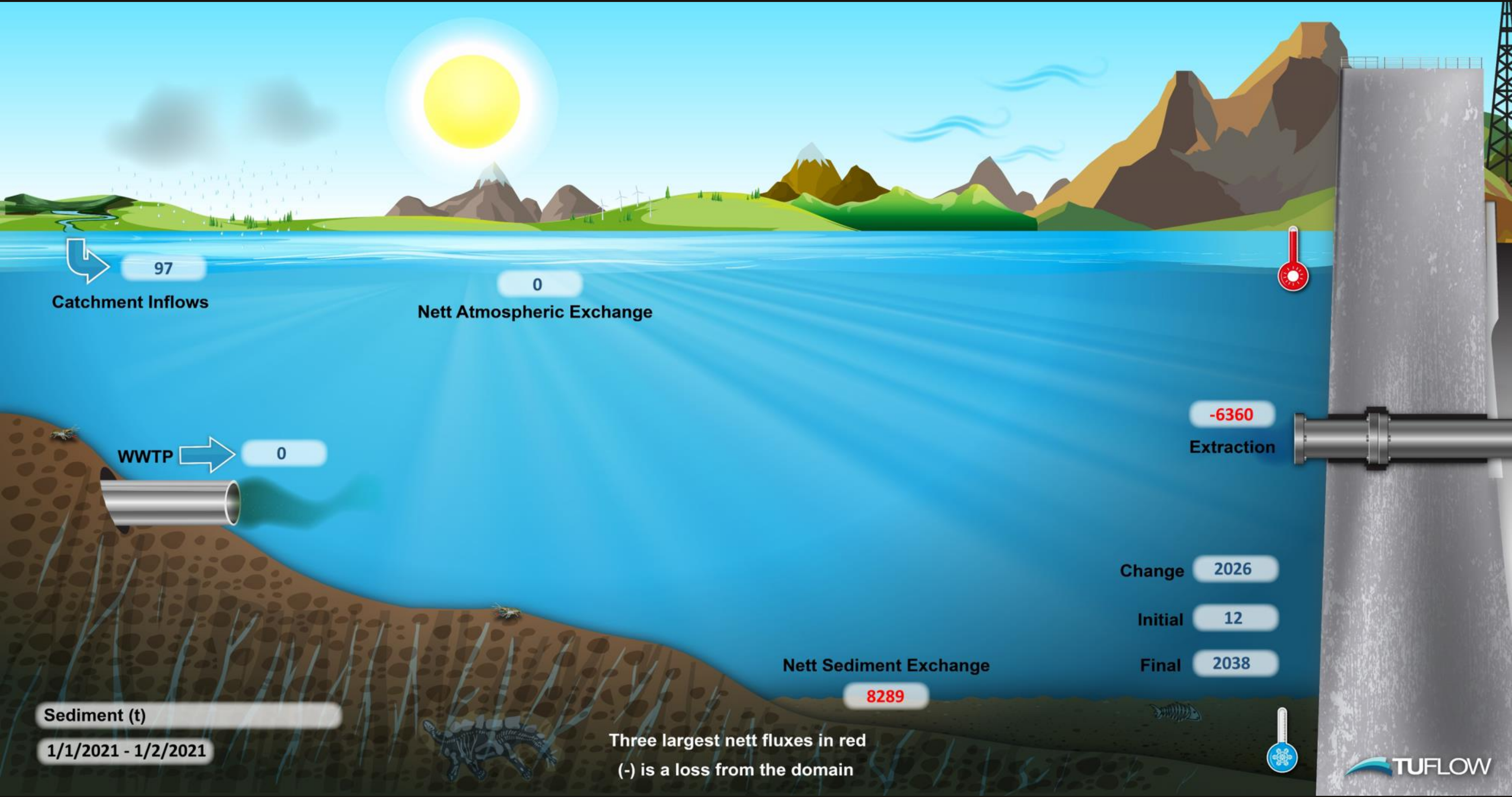
Workshop 1
The review

Sediment

- Solutions
  - Where in the catchment do we work?
  - Integrated model
    allows us to look at fluxes
    (what we are really trying to fix)
  - Examine standing mass and fluxes




Sediment mass: 01-Jan-2021 to 01-Feb-2021
Sediment mass (t Sed)
15000
10000
5000
0
Cumulative boundary Sediment mass fluxes: 01-Jan-2021 to 01-Feb-2021
Cumulative Sediment mass flux (t Sed)
×10^4
1.5
1
0.5
0
-0.5
-1
Surface
WWTP
Benthic
Catchment
Extractions
Internal
Jan 01
Jan 08
Jan 15
Jan 22
Jan 29
Feb 05
Date
2021


97
Catchment Inflows
0
Nett Atmospheric Exchange
-6360
Extraction
WWTP
0
Change
2026
Initial
12
Final
2038
Nett Sediment Exchange
8289
Sediment (t)
1/1/2021 - 1/2/2021
Three largest nett fluxes in red
(-) is a loss from the domain
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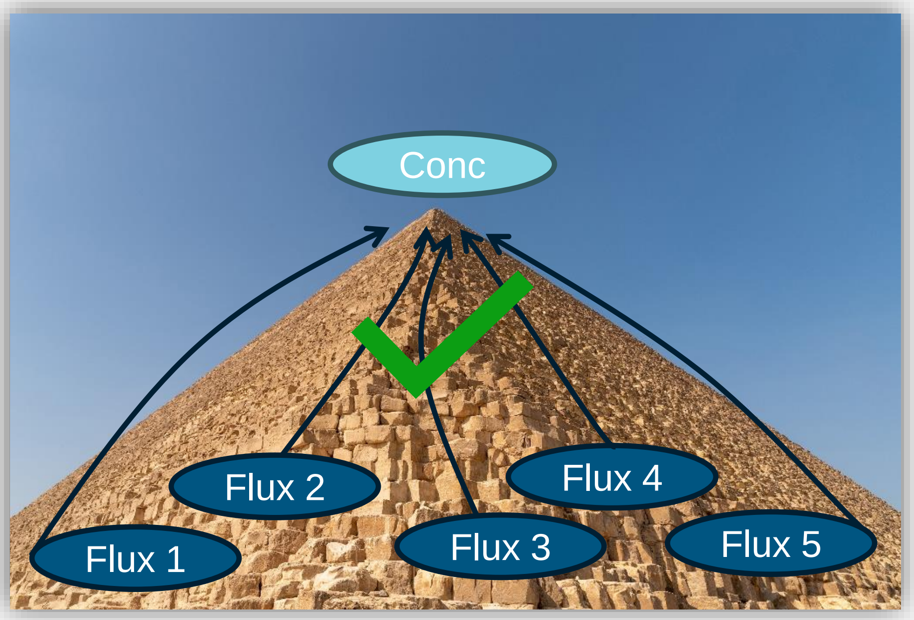
Workshop 1
The review

Sediment

- Solutions
  - Where in the catchment do we work?
  - The rivers!
  - Wasteful scenarios (avoiding disbenefits)
  - Wasteful calibration time
- Sources
  - Ongoing delivery from catchments?
  - Bank erosion? Scour?



The review:
Dissolved oxygen

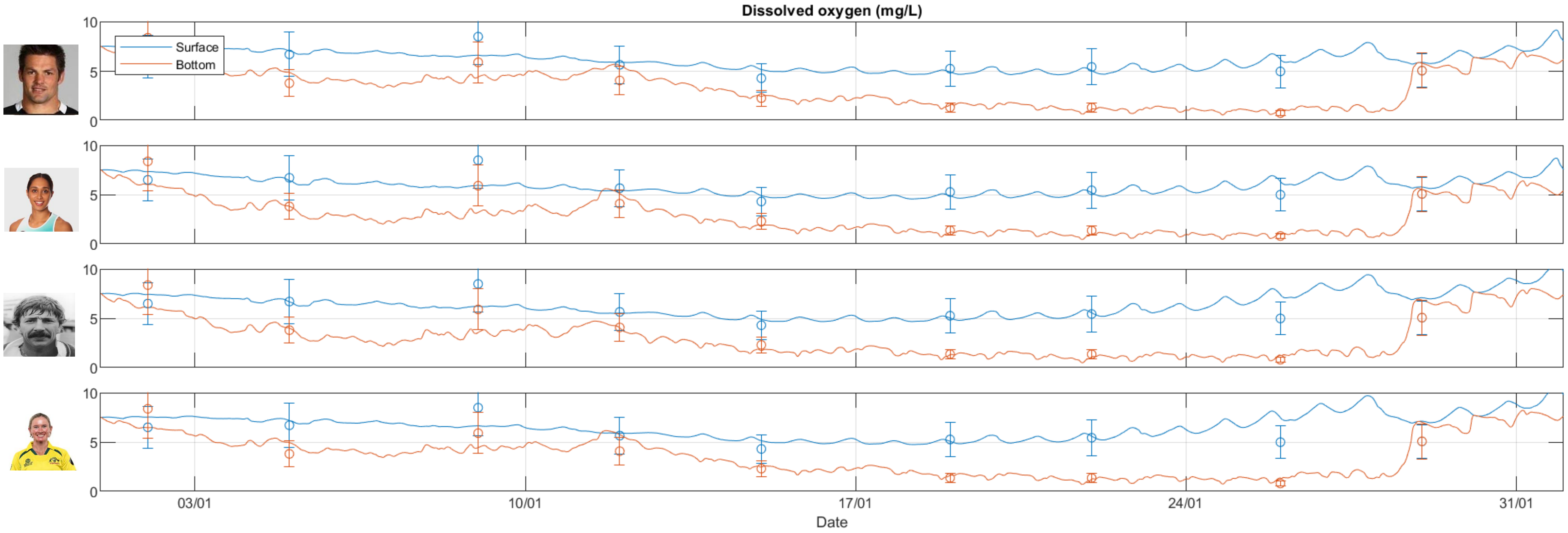
Workshop 1
The review

Dissolved oxygen

- Prediction / calibration of concentrations
- Four modellers
  - Richie
  - Phoenix
  - Rod
  - Beth

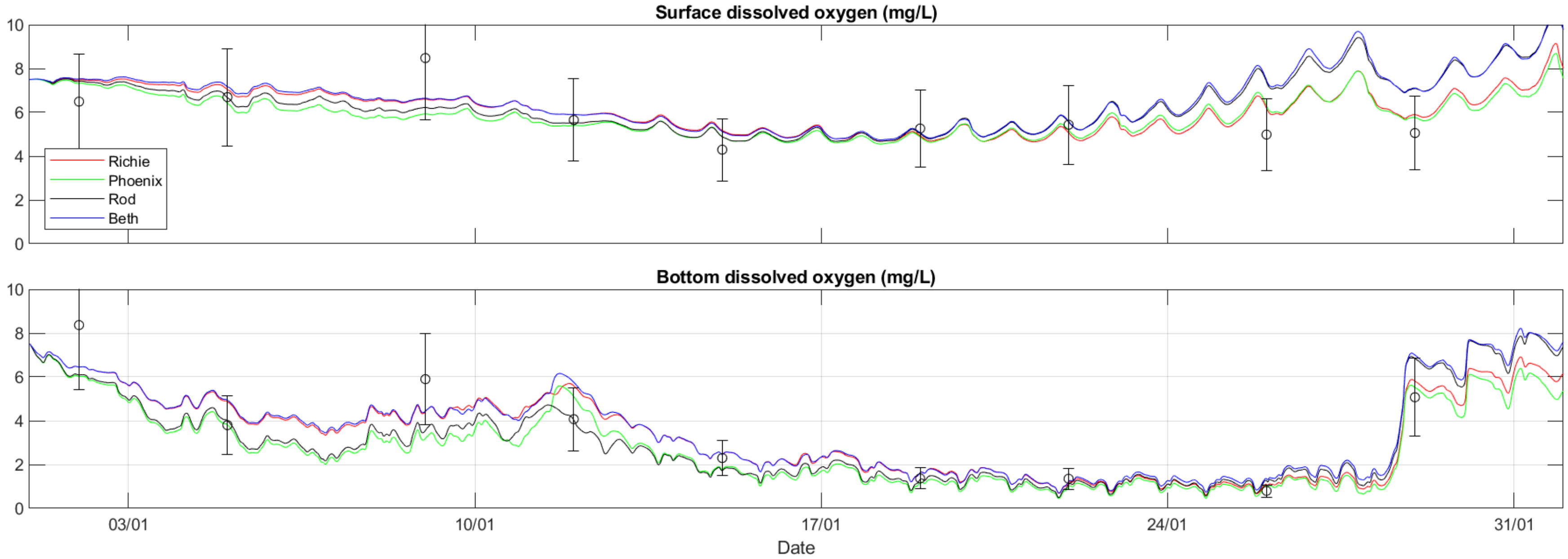
Workshop 1
The review

Dissolved oxygen concentration timeseries



Workshop 1
The review

Dissolved oxygen concentration timeseries



Workshop 1
The review

Dissolved oxygen

- Prediction / calibration of concentrations
- Moriasi 2015
  - Very good
  - Good
  - Satisfactory
  - Not satisfactory

Metric	Richie	Phoenix	Rod	Beth
R	0.89	0.85	0.81	0.83
R^2	0.79	0.72	0.66	0.69
NSE	0.78	0.70	0.63	0.65
IOA	0.93	0.91	0.90	0.90
RMSE	1.0	1.2	1.3	1.3
MAE	0.8	0.8	0.9	1.0
PBIAS	-2.8	5.4	-0.4	-8.8

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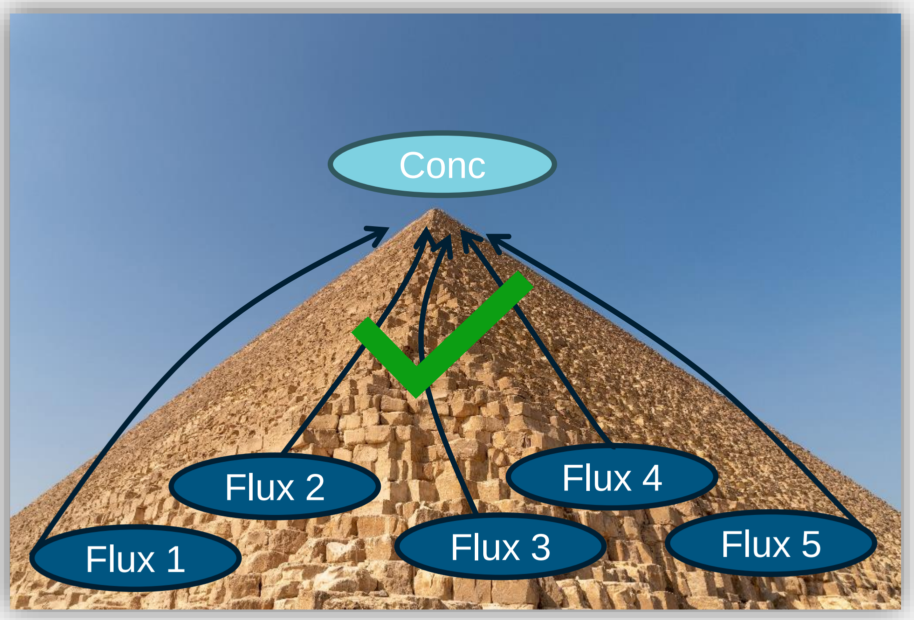
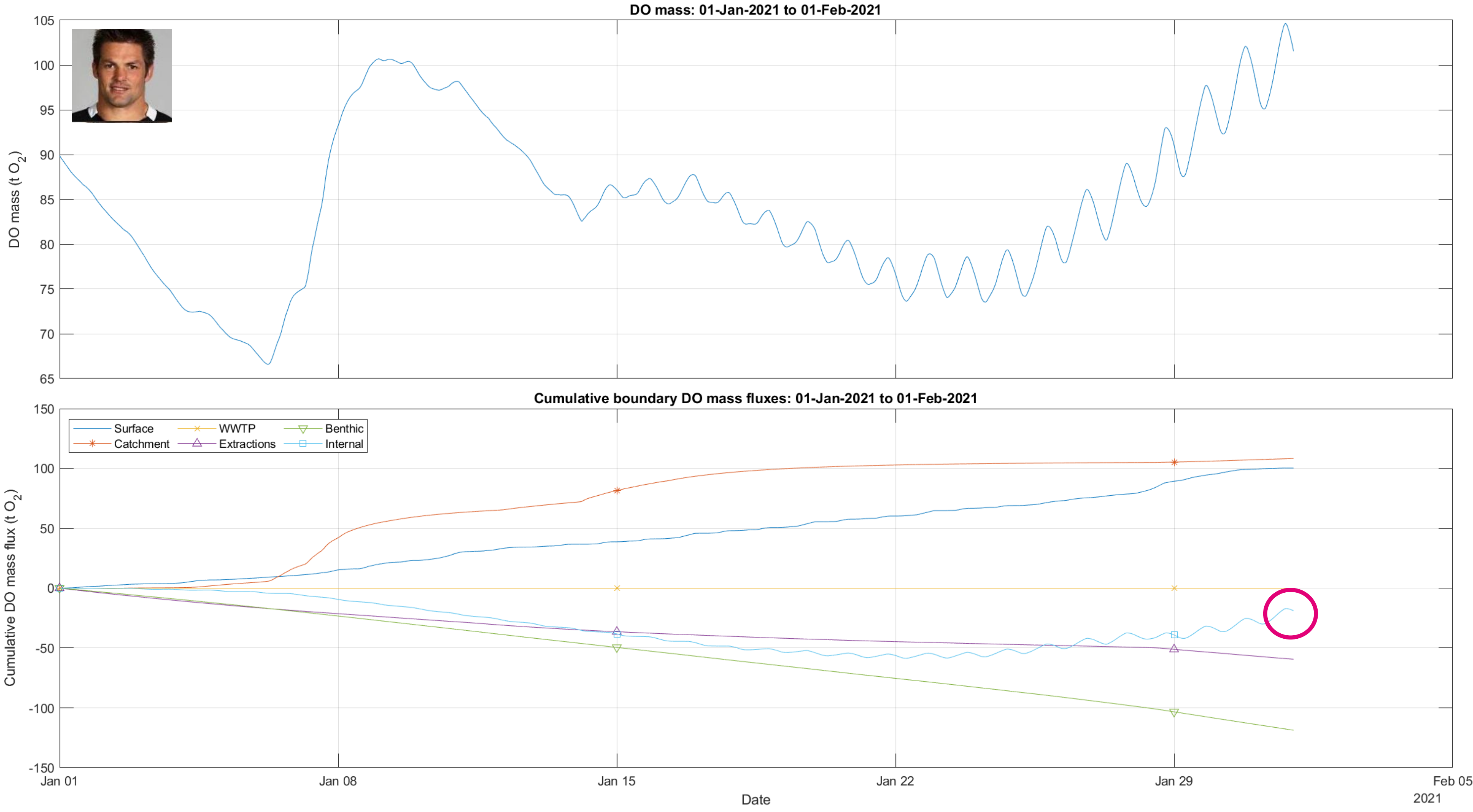
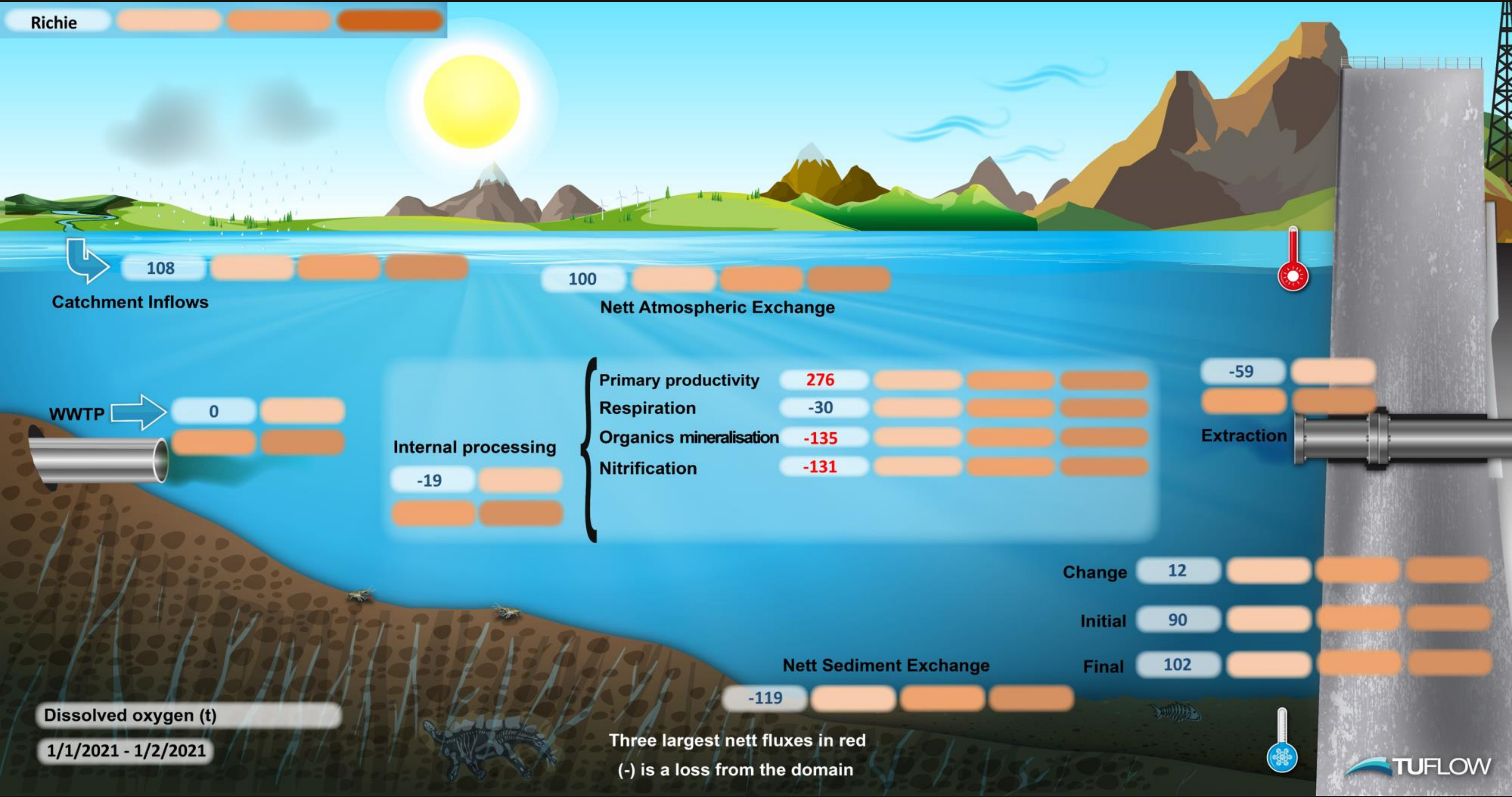
Workshop 1
The review

Dissolved oxygen

- But how to these concentrations come about?
  - TUFLOW FV WQ module reports diagnostics: fluxes of every mass in every process
  - Let's have a look at dissolved oxygen!

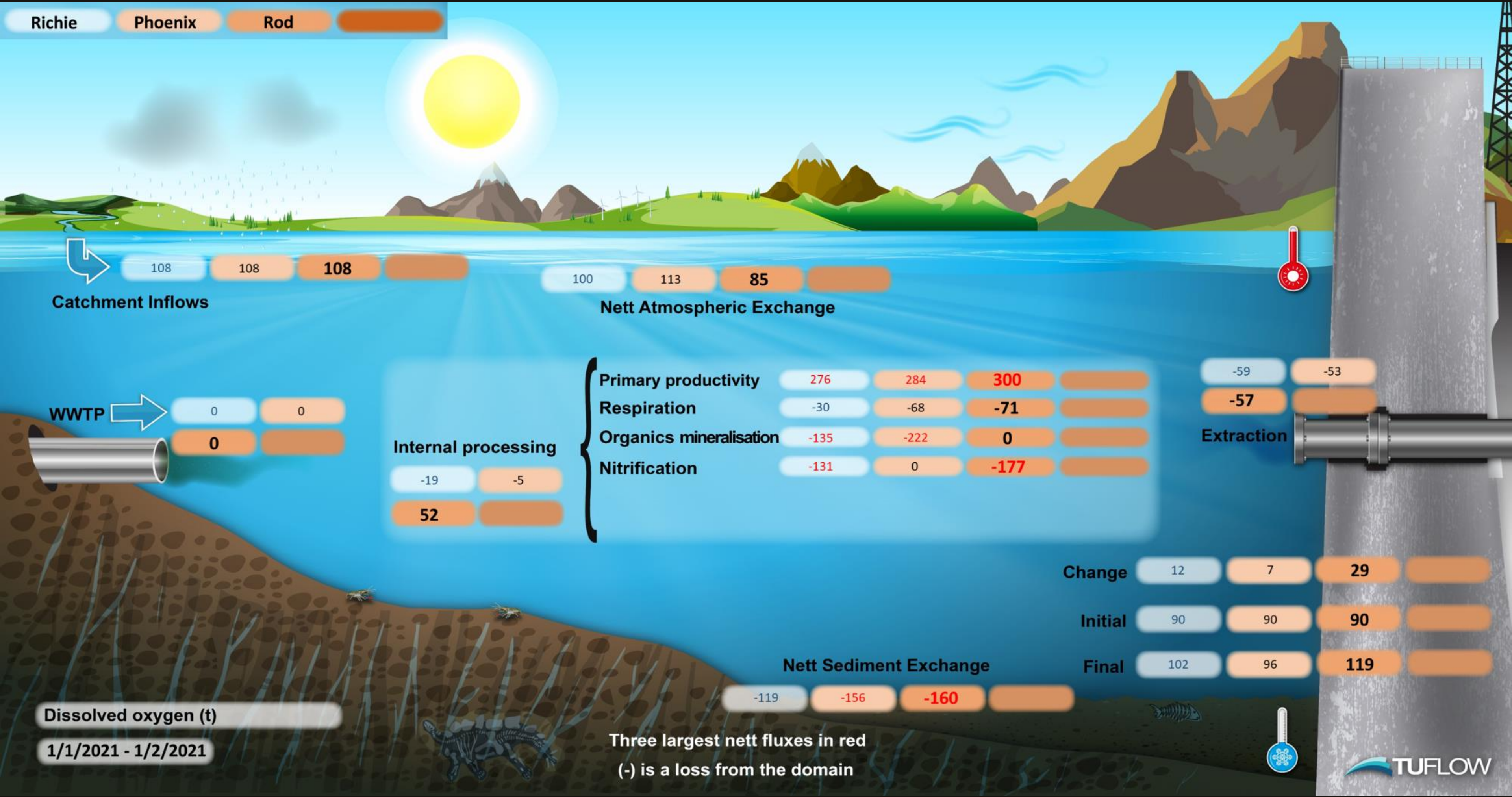



DO mass: 01-Jan-2021 to 01-Feb-2021
DO mass (t O_2)
105
100
95
90
85
80
75
70
65
Cumulative boundary DO mass fluxes: 01-Jan-2021 to 01-Feb-2021
Surface
Catchment
WWTP
Extractions
Benthic
Internal
Cumulative DO mass flux (t O_2)
150
100
50
0
-50
-100
-150
Jan 01
Jan 08
Jan 15
Jan 22
Jan 29
Feb 05
2021
Date

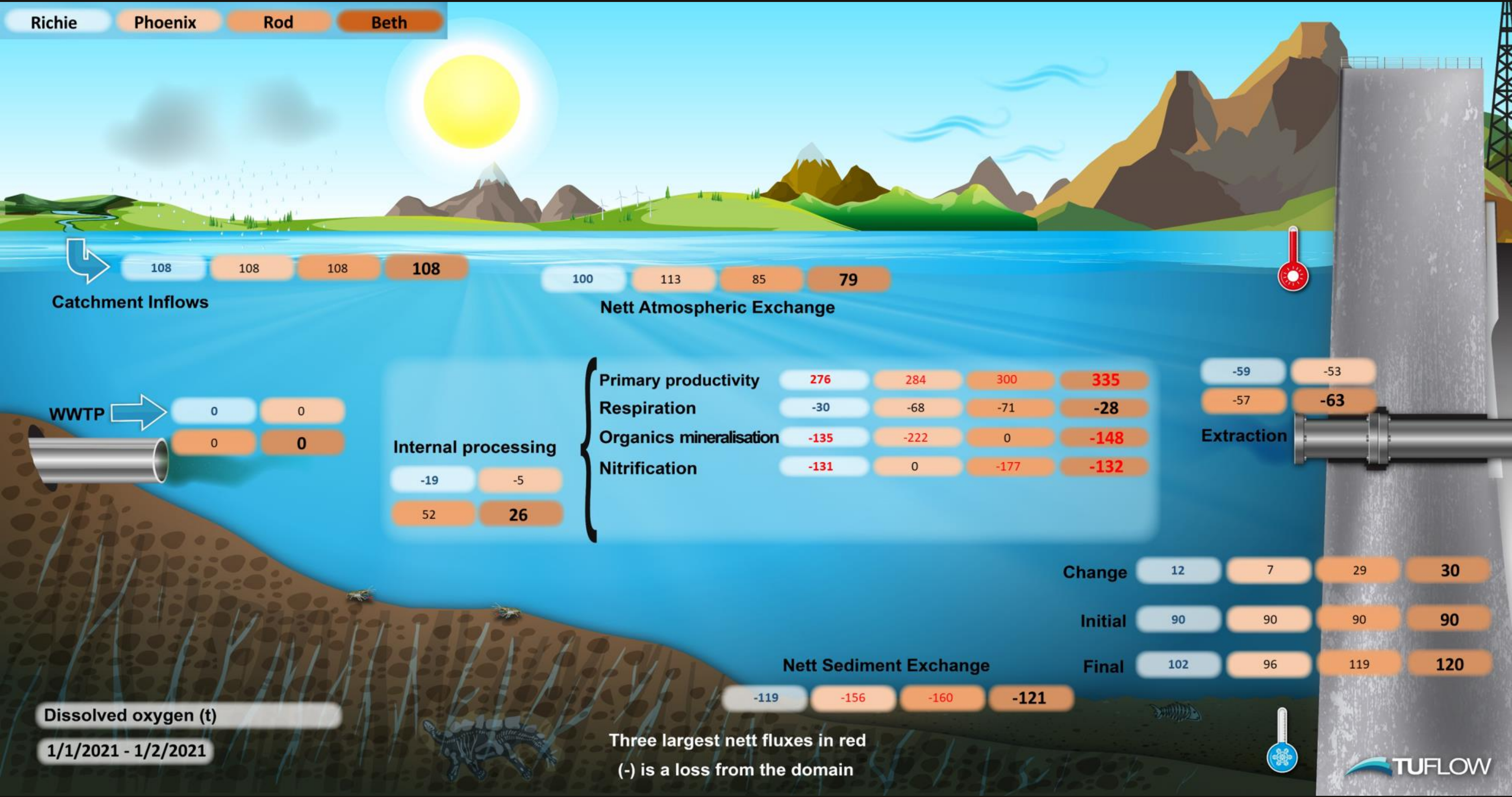


Richie
108
Catchment Inflows
100
Nett Atmospheric Exchange
WWTP
0
Internal processing
-19
Primary productivity
276
Respiration
-30
Organics mineralisation
-135
Nitrification
-131
-59
Extraction
Change
12
Initial
90
Final
102
Nett Sediment Exchange
-119
Dissolved oxygen (t)
1/1/2021 - 1/2/2021
Three largest nett fluxes in red
(-) is a loss from the domain
TUFLOW

Richie
Phoenix
108
108
Catchment Inflows
100
113
Nett Atmospheric Exchange
WWTP
0
0
Internal processing
-19
-5
Primary productivity
276
284
Respiration
-30
-68
Organics mineralisation
-135
-222
Nitrification
-131
0
-59
-53
Extraction
Change
12
7
Initial
90
90
Final
102
96
Nett Sediment Exchange
-119
-156
Dissolved oxygen (t)
1/1/2021 - 1/2/2021
Three largest nett fluxes in red
(-) is a loss from the domain
TUFLOW



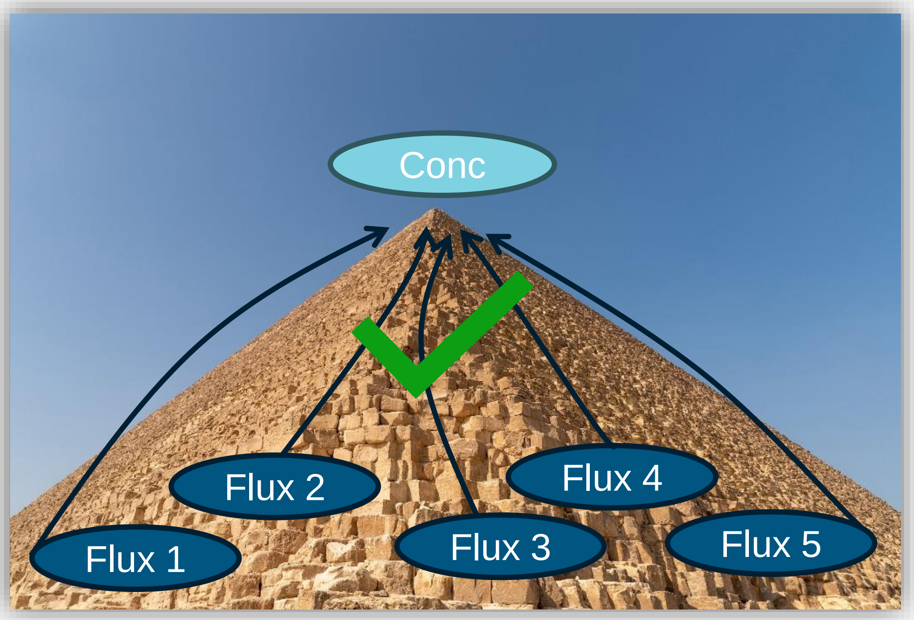
Richie
Phoenix
Rod
108
108
108
Catchment Inflows
100
113
85
Nett Atmospheric Exchange
WWTP
0
0
0
Internal processing
-19
-5
52
Primary productivity
276
284
300
Respiration
-30
-68
-71
Organics mineralisation
-135
-222
0
Nitrification
-131
0
-177
-59
-53
-57
Extraction
Change
12
7
29
Initial
90
90
90
Final
102
96
119
Nett Sediment Exchange
-119
-156
-160
Dissolved oxygen (t)
1/1/2021 - 1/2/2021
Three largest nett fluxes in red
(-) is a loss from the domain
TUFLOW


Richie
Phoenix
Rod
Beth
108
108
108
108
Catchment Inflows
100
113
85
79
Nett Atmospheric Exchange
WWTP
0
0
0
0
Internal processing
-19
-5
52
26
Primary productivity
276
284
300
335
Respiration
-30
-68
-71
-28
Organics mineralisation
-135
-222
0
-148
Nitrification
-131
0
-177
-132
-59
-53
-57
-63
Extraction
Change
12
7
29
30
Initial
90
90
90
90
Final
102
96
119
120
Nett Sediment Exchange
-119
-156
-160
-121
Dissolved oxygen (t)
1/1/2021 - 1/2/2021
Three largest nett fluxes in red
(-) is a loss from the domain
TUFLOW

Workshop 1
The review

Dissolved oxygen

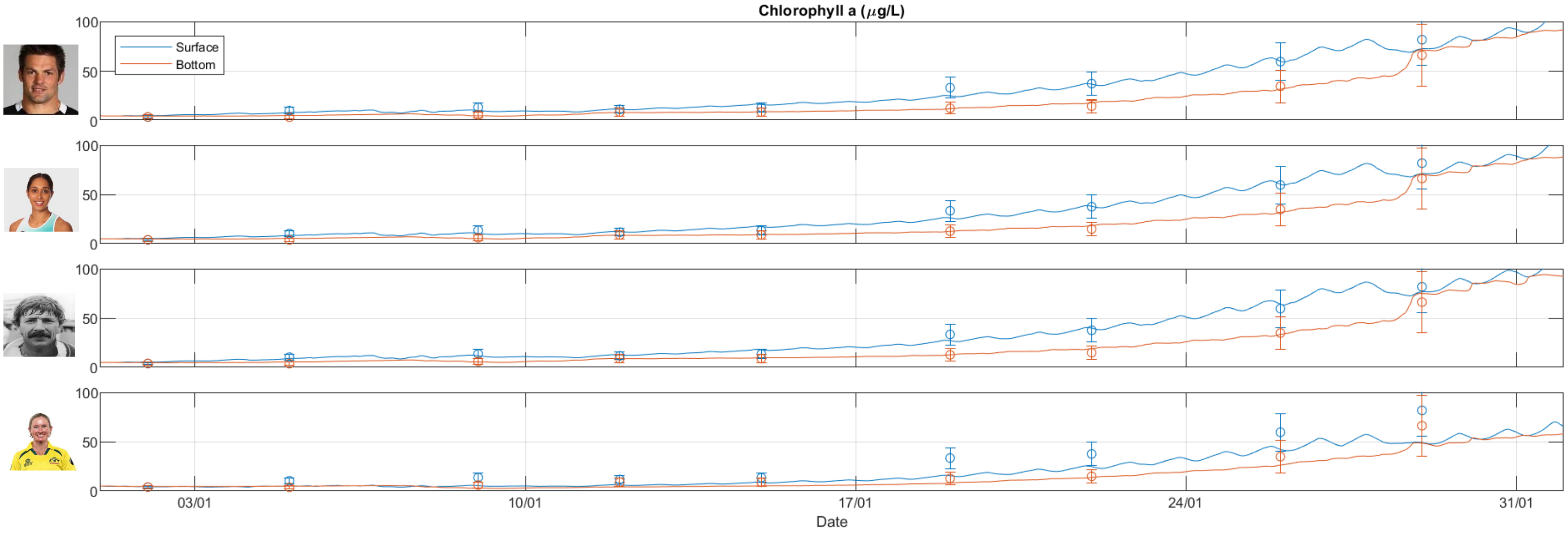
- Solutions
  - Our modellers have the right answers for the wrong reasons!
  - So what do we do?
- Engage and understand via flux diagnostics discussion to understand
  - Managers and decision makers
  - Traditional owners
  - …



The review:
Chlorophyll a

Workshop 1
The review

Chlorophyll a



Workshop 1
The review

Chlorophyll a

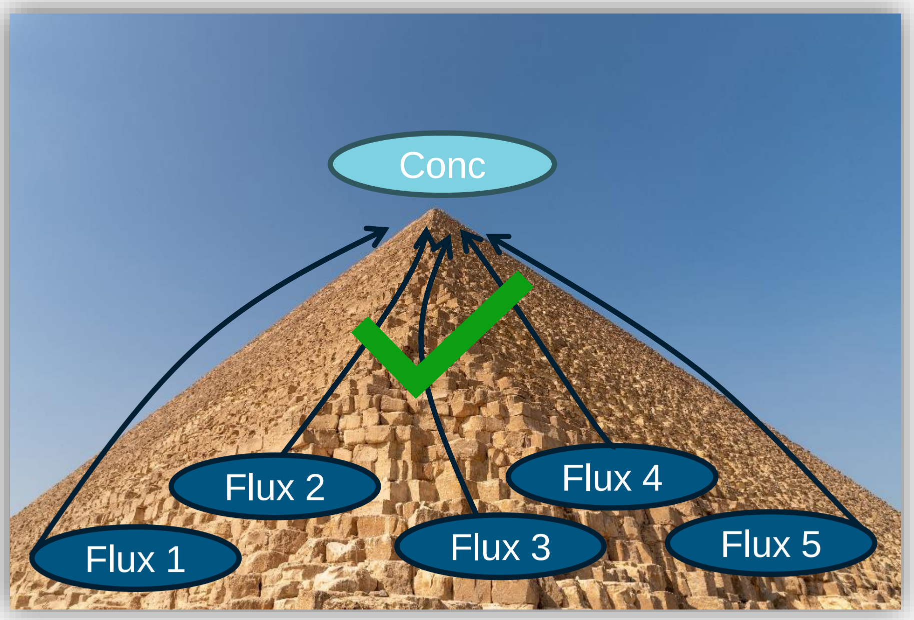
- Prediction / calibration of concentrations
- Moriasi 2015
  - Very good
  - Good
  - Satisfactory
  - Not satisfactory

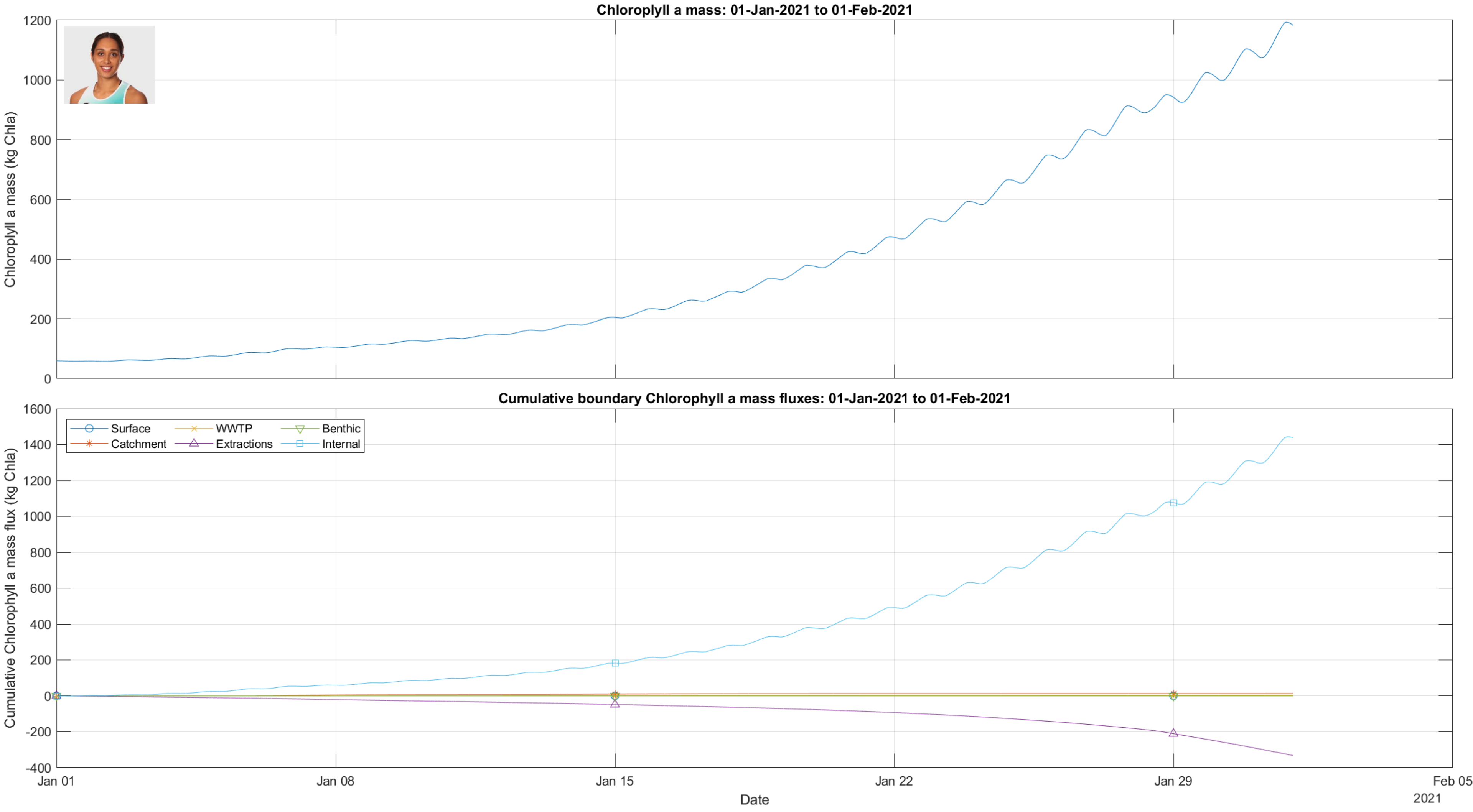
Metric	Richie	Phoenix	Rod	Beth
R	0.99	0.99	0.98	0.98
R^2	0.98	0.98	0.97	0.96
NSE	0.97	0.97	0.98	0.77
IOA	0.99	0.99	0.99	0.91
RMSE	3.5	3.6	3.5	11.6
MAE	2.4	2.4	2.5	8.3
PBIAS	2.5	2.3	-3.0	34

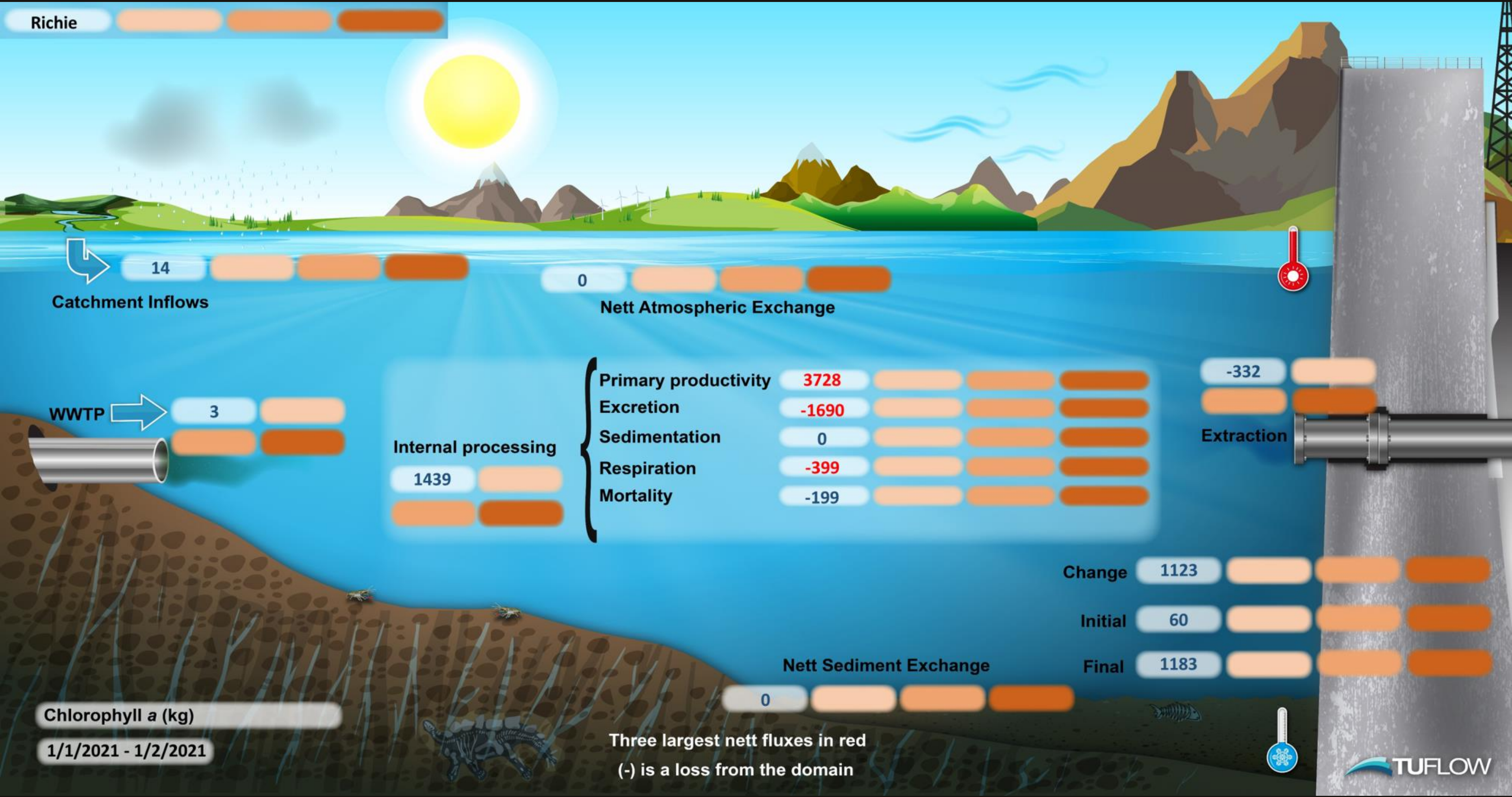
Workshop 1
The review

Dissolved oxygen

- But how to these concentrations come about?
  - TUFLOW FV WQ module reports diagnostics: fluxes of every mass in every process
  - Let’s have a look at chlorophyll a!




Chloroplyll a mass: 01-Jan-2021 to 01-Feb-2021
Chloroplyll a mass (kg Chla)
0
200
400
600
800
1000
1200
Cumulative boundary Chlorophyll a mass fluxes: 01-Jan-2021 to 01-Feb-2021
Cumulative Chlorophyll a mass flux (kg Chla)
-400
-200
0
200
400
600
800
1000
1200
1400
1600
Surface
Catchment
WWTP
Extractions
Benthic
Internal
Jan 01
Jan 08
Jan 15
Jan 22
Jan 29
Feb 05
2021
Date



Richie
14
Catchment Inflows
0
Nett Atmospheric Exchange
WWTP
3
Internal processing
1439
Primary productivity 3728
Excretion -1690
Sedimentation 0
Respiration -399
Mortality -199
-332
Extraction
Change 1123
Initial 60
Final 1183
Nett Sediment Exchange
0
Chlorophyll a (kg)
1/1/2021 - 1/2/2021
Three largest nett fluxes in red
(-) is a loss from the domain
TUFLOW

Richie
Phoenix
14
14
Catchment Inflows
0
0
Nett Atmospheric Exchange
WWTP
3
3
Internal processing
1439
1388
Primary productivity
3728
3835
Excretion
-1690
-1534
Sedimentation
0
0
Respiration
-399
-913
Mortality
-199
0
-332
-327
Extraction
Change
1123
1078
Initial
60
60
Final
1183
1137
Nett Sediment Exchange
0
0
Chlorophyll a (kg)
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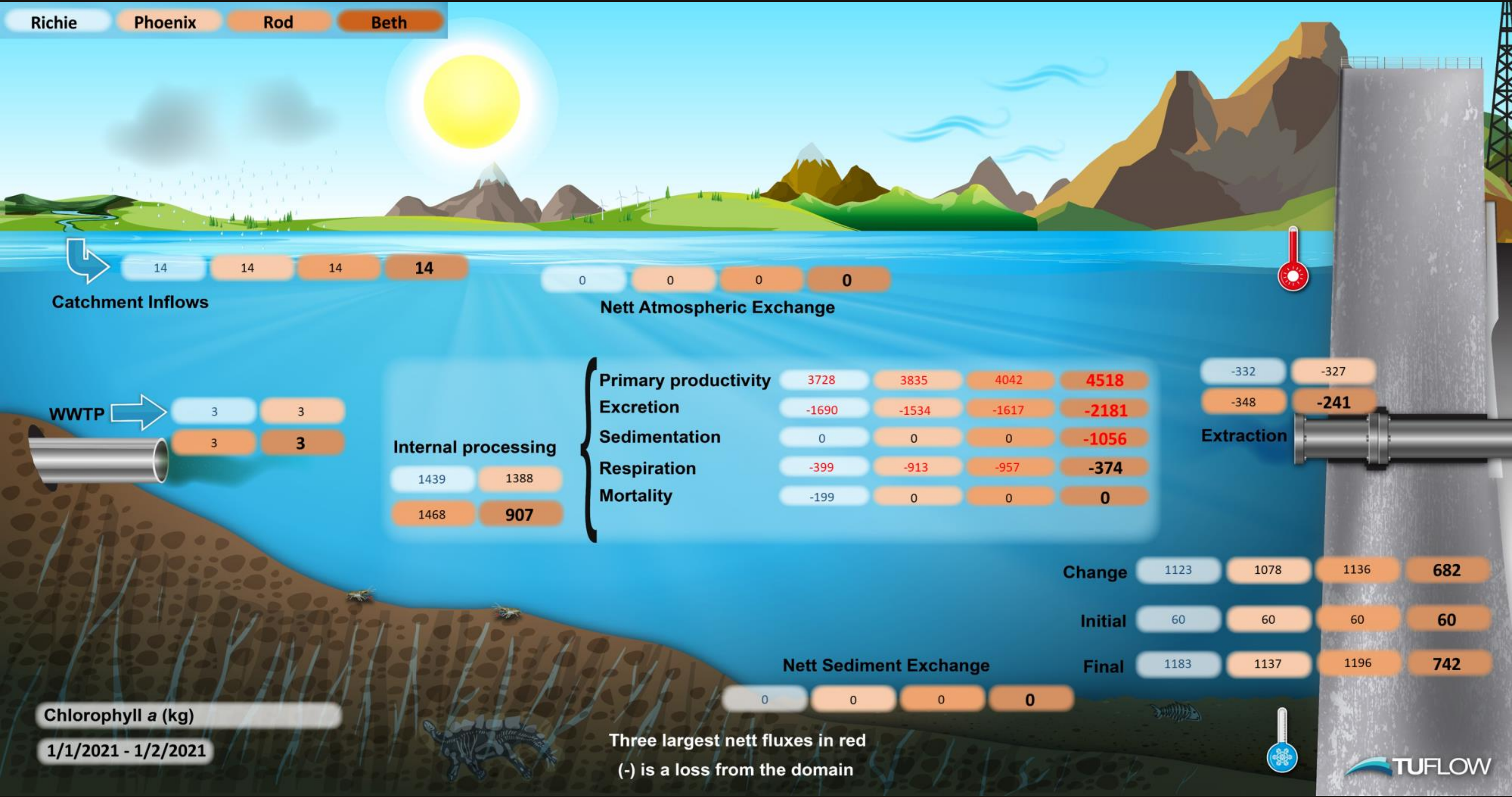
TUFLOW

Richie
Phoenix
Rod
14
14
14
Catchment Inflows
0
0
0
Nett Atmospheric Exchange
WWTP
3
3
3
Internal processing
1439
1388
1468
Primary productivity
3728
3835
4042
Excretion
-1690
-1534
-1617
Sedimentation
0
0
0
Respiration
-399
-913
-957
Mortality
-199
0
0
-332
-327
-348
Extraction
Change
1123
1078
1136
Initial
60
60
60
Final
1183
1137
1196
Nett Sediment Exchange
0
0
0
Chlorophyll a (kg)
1/1/2021 - 1/2/2021
Three largest nett fluxes in red
(-) is a loss from the domain
TUFLOW

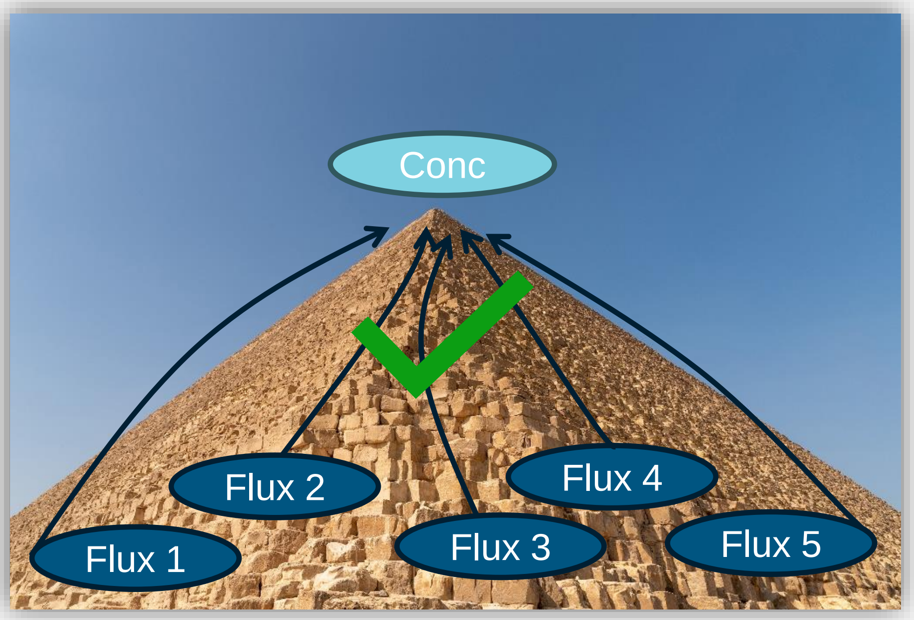


Richie
Phoenix
Rod
Beth
Catchment Inflows
14
14
14
14
Nett Atmospheric Exchange
0
0
0
0
WWTP
3
3
3
3
Internal processing
1439
1388
1468
907
Primary productivity
3728
3835
4042
4518
Excretion
-1690
-1534
-1617
-2181
Sedimentation
0
0
0
-1056
Respiration
-399
-913
-957
-374
Mortality
-199
0
0
0
Extraction
-332
-327
-348
-241
Change
1123
1078
1136
682
Initial
60
60
60
60
Final
1183
1137
1196
742
Nett Sediment Exchange
0
0
0
0
Chlorophyll a (kg)
1/1/2021 - 1/2/2021
Three largest nett fluxes in red
(-) is a loss from the domain
TUFLOW

Workshop 1
The review

Chlorophyll a

- Solutions
  - Our modellers have good enough answers for the wrong reasons!
  - Which one is more correct, if any?
- As with DO
  - Time to engage
  - Managers and decision makers
  - Traditional owners

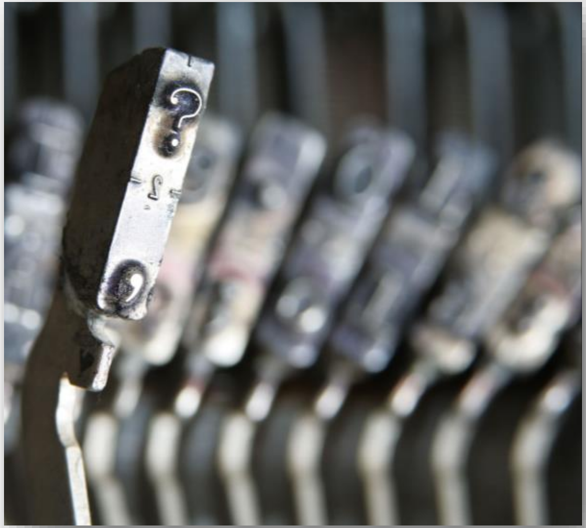


The verdict

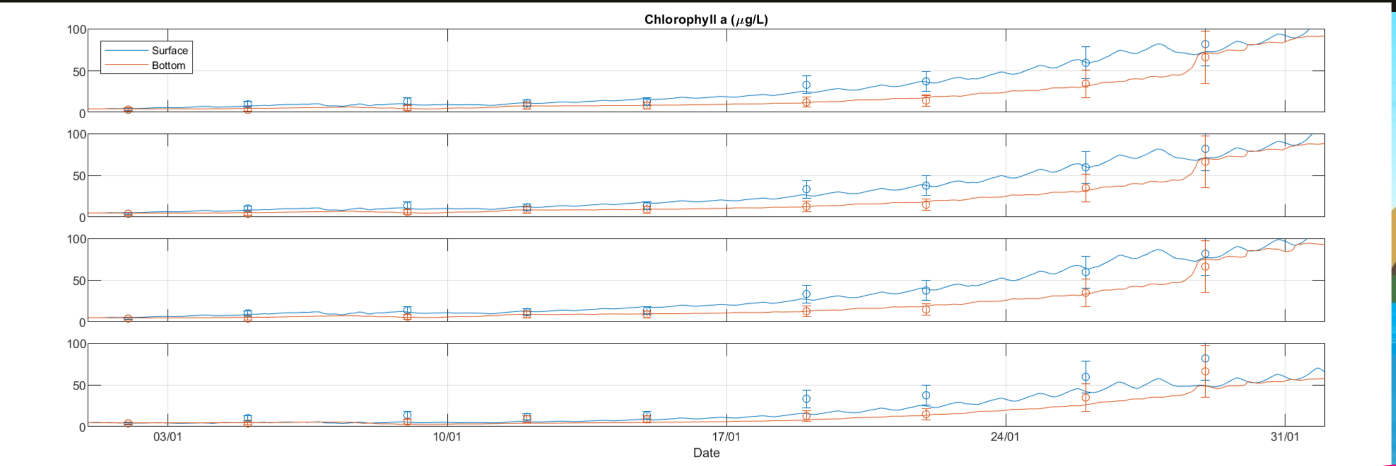
Workshop 1
The verdict

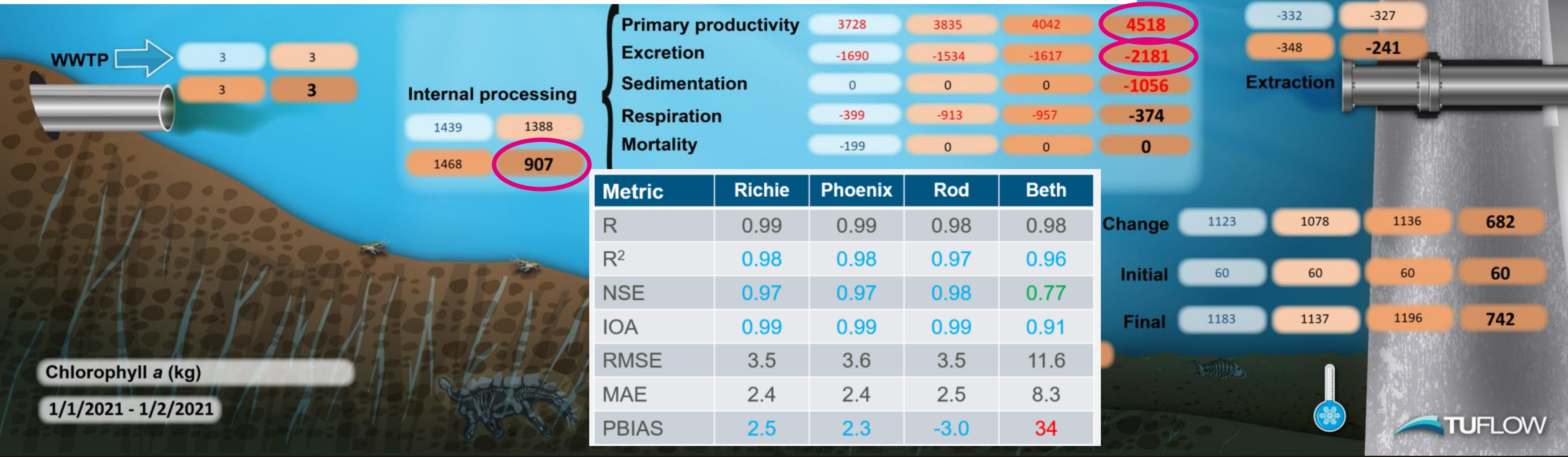
Declan

- 50 years living in the catchment and working at the treatment plant
  - It is very poor in organics
  - Sludge exists at the bottom of the reservoir
  - Urbanisation has made green blooms much worse
  - Nitrates are high at the downstream water treatment plant
- Who does Declan go with?
- As peer reviewers – what do you now do?



The wrap



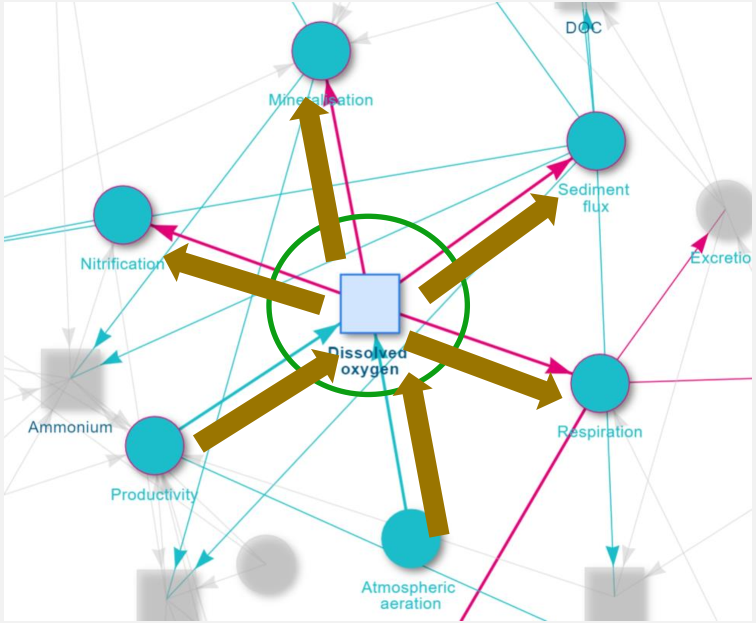


Metric	Richie	Phoenix	Rod	Beth
R	0.99	0.99	0.98	0.98
R^2	0.98	0.98	0.97	0.96
NSE	0.97	0.97	0.98	0.77
IOA	0.99	0.99	0.99	0.91
RMSE	3.5	3.6	3.5	11.6
MAE	2.4	2.4	2.5	8.3
PBIAS	2.5	2.3	-3.0	34

Workshop 1
The wrap

Outcomes

- Simulation, modelling and analysis of the living water system:
  Improving our beneficial return on investment
- Models offer richness of data
- Compliance (past and future)
  - Timeseries (necessary but not sufficient)
  - Statistics (necessary but not sufficient)
- Understanding and beneficial return (future)
  - Fluxes (should be mandatory)



Workshop 1
The wrap

Concentrations and fluxes

- Not new
  - Hipsey et al. (2020)

ELSEVIER

Environmental Modelling & Software
Volume 128, June 2020, 104697

A system of metrics for the assessment and improvement of aquatic ecosystem models

Matthew R. Hipsey [a b], Gideon Gal [c], George B. Arhonditsis [d], Cayelan C. Carey [e], J. Alex Elliott [f], Marieke A. Frassl [g], Jan H. Janse [h], Lee de Mora [i], Barbara J. Robson [j]

Workshop 1
The wrap

Concentrations and fluxes

- Comparing model concentration timeseries with point field measurements (or medians, or by zones) actively excludes understanding
  - Wasteful scenarios (avoiding disbenefits)
  - Wasteful calibration time – often the major project and community resource sink
  - Get the right answers for the wrong reasons
  - End up arguing over modelled timeseries and measured points not matching

Workshop 1
The wrap

Concentrations and fluxes

- Understanding mass fluxes through environmental systems is essential to effective management
  - This is the substantial opportunity to improve on the beneficial return on investment we make in the living water system

Thank you

Appendix:
Background science

Workshop 1
Background science

Internal processes – dissolved oxygen

- Atmospheric exchange (https://docs.tuflow.com/fv/wqm/manual/2023/AppO.html#AtmosphericAeration-3)

Atmospheric oxygen flux is a key source of water column dissolved oxygen. Oxygenation is implemented in the upper model layer by the WQ Module, and then this oxygenated water is mixed downwards by TUFLOW in subsequent timesteps.

Initially, a Schmidt number $Sc^{O_2}_{atm}$ is computed via Equation (D.1).

$$Sc^{O_2}_{atm} = \left(0.9 + \frac{S}{350.0}\right) \times \left(2073.1 - 125.62T + 3.6276T^2 - 0.043219T^3\right) \quad (D.1)$$

T and S are ambient water temperature and salinity respectively. An oxygen piston velocity $V^{O_2}_{pist}$ (also known as a gas transfer velocity) is then computed. Two piston models for $V^{O_2}_{pist}$ are available. The first is due to Wanninkhof (1992):

$$V^{O_2}_{pist} = 0.31\left(V^{O_2}_{wind}\right)^2 \times \left(\frac{660.0}{Sc^{O_2}_{atm}}\right)^x \quad (D.2)$$

where $V^{O_2}_{wind}$ is wind speed. For wind speed $V^{O_2}_{wind}$<3.0 m/s, x is 0.66, otherwise x is 0.5. Wind speed is assumed to be provided from TUFLOW at 10 metres from the water surface. The second is due to Ho et al. (2016):

$$V^{O_2}_{pist} = \left(0.77\sqrt{\frac{V_{water}}{H_{layer}}} + 0.266\left(V^{O_2}_{wind}\right)^2\right) \times \sqrt{\frac{660.0}{Sc^{O_2}_{atm}}} \quad (D.3)$$

where V_{water} is surface water speed, H_{layer} is the thickness of the uppermost TUFLOW FV computational layer and $V^{O_2}_{wind}$ is wind speed.

There are other models available for computing both $Sc^{O_2}_{atm}$ and $V^{O_2}_{pist}$ within the WQ Module. Contact support@tuflow.com if these are required.

Once $Sc^{O_2}_{atm}$ and $V^{O_2}_{pist}$ are known, oxygenation to the surface layer is computed as per Equation (D.4).

$$F^{O_2}_{atm} = V^{O_2}_{pist}\left([DO]_{air} - [DO]\right) \quad (D.4)$$

Workshop 1
Background science

Internal processes – dissolved oxygen

- Sediment flux (https://docs.tuflow.com/fv/wqm/manual/2023/AppO.html#SedOxyCons-3)

Oxygen is exchanged between the water column and sediments via specification of a sediment flux representing the net effect of biological activity. In the case of oxygen, this flux is most commonly into the sediments, i.e. a negative sediment flux. Although it is rare that sediments act as sources of oxygen, the WQ Module can be parameterised to allow for this if required.

The user specified sediment oxygen flux (which can be spatially varying) is modified by overlying ambient dissolved oxygen concentration (together with a user specified half saturation oxygen concentration) and water temperature. These modifications are simulated via Michaelis-Menten and Arrhenius models, respectively, as per Equation (D.6).

$$F^{O_2}_{sed\langle computed\rangle} = F^{O_2}_{sed} \times \underbrace{\frac{[DO]}{K^{O_2}_{sed-O_2} + [DO]}}_{\text{Influence of oxygen}} \times \underbrace{\left[\theta^{O_2}_{sed}\right]^{(T-20)}}_{\text{Influence of temperature}} \qquad \text{(D.6)}$$

$F^{O_2}_{sed}$ is the user specified oxygen sediment flux at 20^{o}C without the influence of dissolved oxygen, $[DO]$ is the overlying dissolved oxygen concentration computed by the WQ Module, $K^{O_2}_{sed-O_2}$ and $\theta^{O_2}_{sed}$ are the half saturation oxygen concentration and temperature coefficient for dissolved oxygen sediment flux respectively, and T is ambient water temperature.

Workshop 1
Background science

Internal processes – dissolved oxygen

- Primary productivity (https://docs.tuflow.com/fv/wqm/manual/2023/PhyRates-3.html#PhyProd-4)
  - Primary productivity is the consumption of carbon and the generation of oxygen and carbohydrate due to photosynthesis. Photosynthetically active radiation catalyses this process so it occurs only during daylight hours. This process is also referred to as growth or gross primary productivity

$$C + O_2 \leftarrow CO_2$$

- Respiration (https://docs.tuflow.com/fv/wqm/manual/2023/PhyRates-3.html#PhyResp-4)
  - Respiration is the consumption of oxygen and stored carbohydrate and the production of carbon. This can be thought of as the reverse of primary productivity. Respiration dominates phytoplankton dynamics during nighttime hours, although it generally still operates during the daytime

$$C + O_2 \rightarrow CO_2$$

Workshop 1
Background science

Internal processes – dissolved oxygen

- Organics mineralisation (https://docs.tuflow.com/fv/wqm/manual/2023/AppOrg.html#Miner-3)

Mineralisation is the pelagic biological conversion of labile dissolved organic matter to dissolved inorganic carbon and nutrients. It is therefore a source of dissolved inorganic carbon, ammonium and filterable reactive phosphorus, and a sink of the corresponding labile dissolved organics. Mineralisation is conceptualised as comprising aerobic (i.e. consuming dissolved oxygen and (via denitrification) inorganic nitrate) and anaerobic components, and is implemented within the labile organics constituent model of the WQ Module.

- Nitrification (https://docs.tuflow.com/fv/wqm/manual/2023/AppOrg.html#Miner-3)

Nitrification is the pelagic biological oxidation of ammonium to nitrate. The equations representing this process (including intermediates) are as follows.

$$\left.\begin{array}{l} 2NH_4^+ + 3O_2 \rightarrow 2NO_2^- + 4H^+ + 2H_2O \\ 2NO_2^- + O_2 \rightarrow 2NO_3^- \end{array}\right\}$$

Workshop 1
Background science

Internal processes – phytoplankton

- Primary productivity (https://docs.tuflow.com/fv/wqm/manual/2023/PhyRates-3.html#PhyProd-4)
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$$C + O_2 \rightarrow CO_2$$

Workshop 1
Background science

Internal processes – phytoplankton

- Excretion (https://docs.tuflow.com/fv/wqm/manual/2023/PhyLosses-3.html#PhyLossC-4)

Excretion loss: Computed from a combination of respiration and exudation rates ($R^{phy}_{resp\langle computed\rangle}$ and $R^{phy}_{exud\langle computed\rangle}$, respectively)

$$F^{phy}_{C-excr} = \left(\left[\left(1 - f^{phy}_{true-resp}\right) \times f^{phy}_{excr-loss} \times R^{phy}_{resp\langle computed\rangle}\right] + R^{phy}_{exud\langle computed\rangle}\right) \times [PHY]$$

- Mortality (https://docs.tuflow.com/fv/wqm/manual/2023/PhyLosses-3.html#PhyLossC-4)

Mortality loss: Computed from the respiration rate $R^{phy}_{resp\langle computed\rangle}$

$$F^{phy}_{C-mort} = \left(\left(1 - f^{phy}_{true-resp}\right) \times \left(1 - f^{phy}_{excr-loss}\right) \times R^{phy}_{resp\langle computed\rangle}\right) \times [PHY]$$

Appendix:
References

Workshop 1
References

Publications

- M. Hipsey, G. Gal, G. Arhonditsis, C. Carey, J. A. Elliott, M. Frassl, J. Janse, L. de Mora and B. Robson (2020) “A system of metrics for the assessment and improvement of aquatic ecosystem models”, Environmental Modelling & Software **128**
- D. Moriasi, M. Gitau, N. Pai and P. Daggupati (2015) “Hydrologic and water quality models: performance measures and evaluation criteria”, Transactions of the ASABE **58**:1763-1785
- D. Moriasi, J. Arnold, M. Van Liew, R. Bingner, R. Harmel and T. Veith (2007) “Model evaluation guidelines for systematic quantification of accuracy in watershed simulations”, Transactions of the ASABE **50**