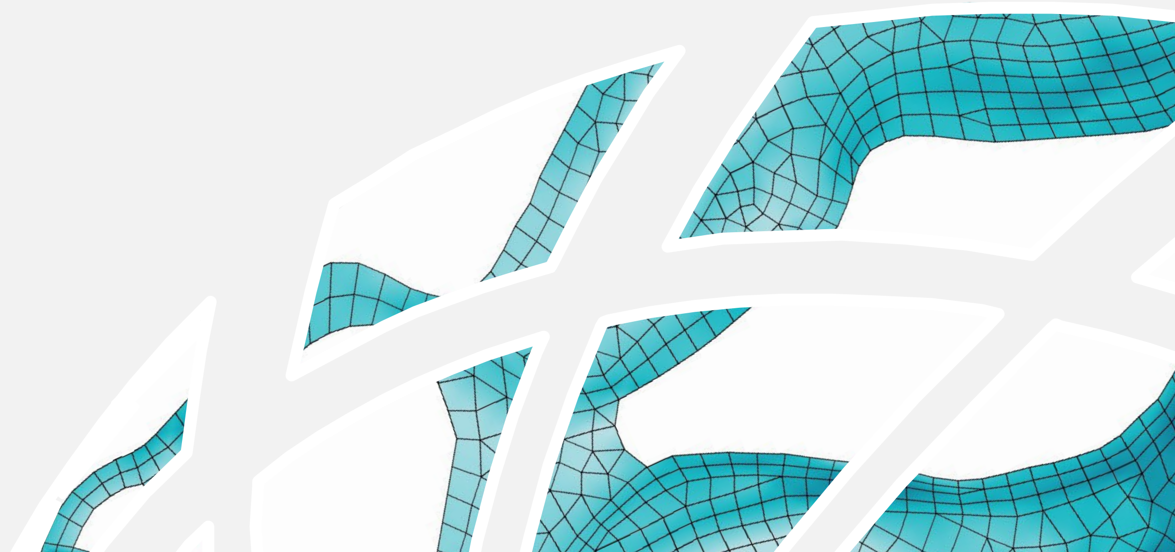
Water quality model validation using mass balance analysis

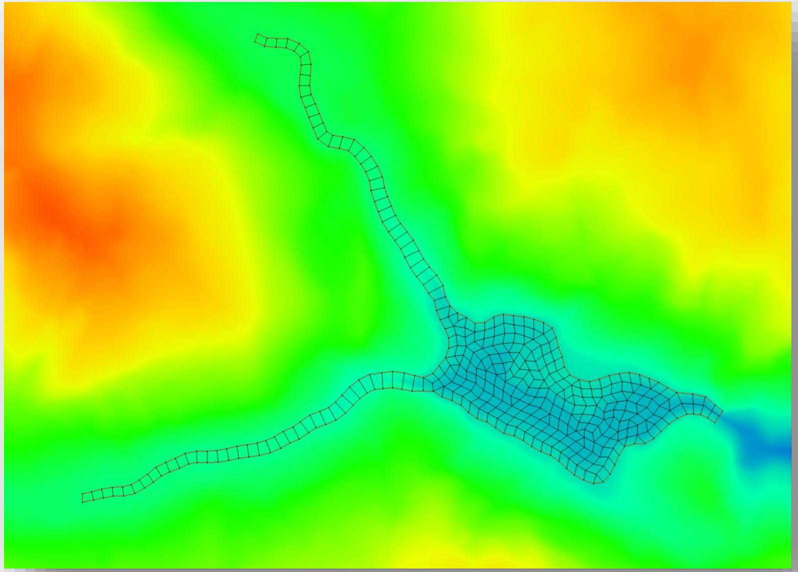


17th April 2024

Agenda

We'll cover

- Context – concentrations and fluxes
- Explore through a hypothetical "calibration"
  - Dissolved oxygen
- Key messages and wrap



Context

Water quality modelling

- What I often hear:
  - Too hard
  - Too many parameters
  - Where do I start?
  - Black box of magic tricks
  - Hocus pocus abracadabra
  - How do I know my model is robust?

Context

Water quality modelling

- Why?
  - We can easily get the 'right answers for the wrong reasons', if
  - The 'right answers' means numerical models can predict 'the same' water quality **concentrations** (C) as measured **concentrations**

A concentration is typically a mass per unit volume of water

Dissolved oxygen concentrations are in milligrams of oxygen per litre 'mg/L'

Context

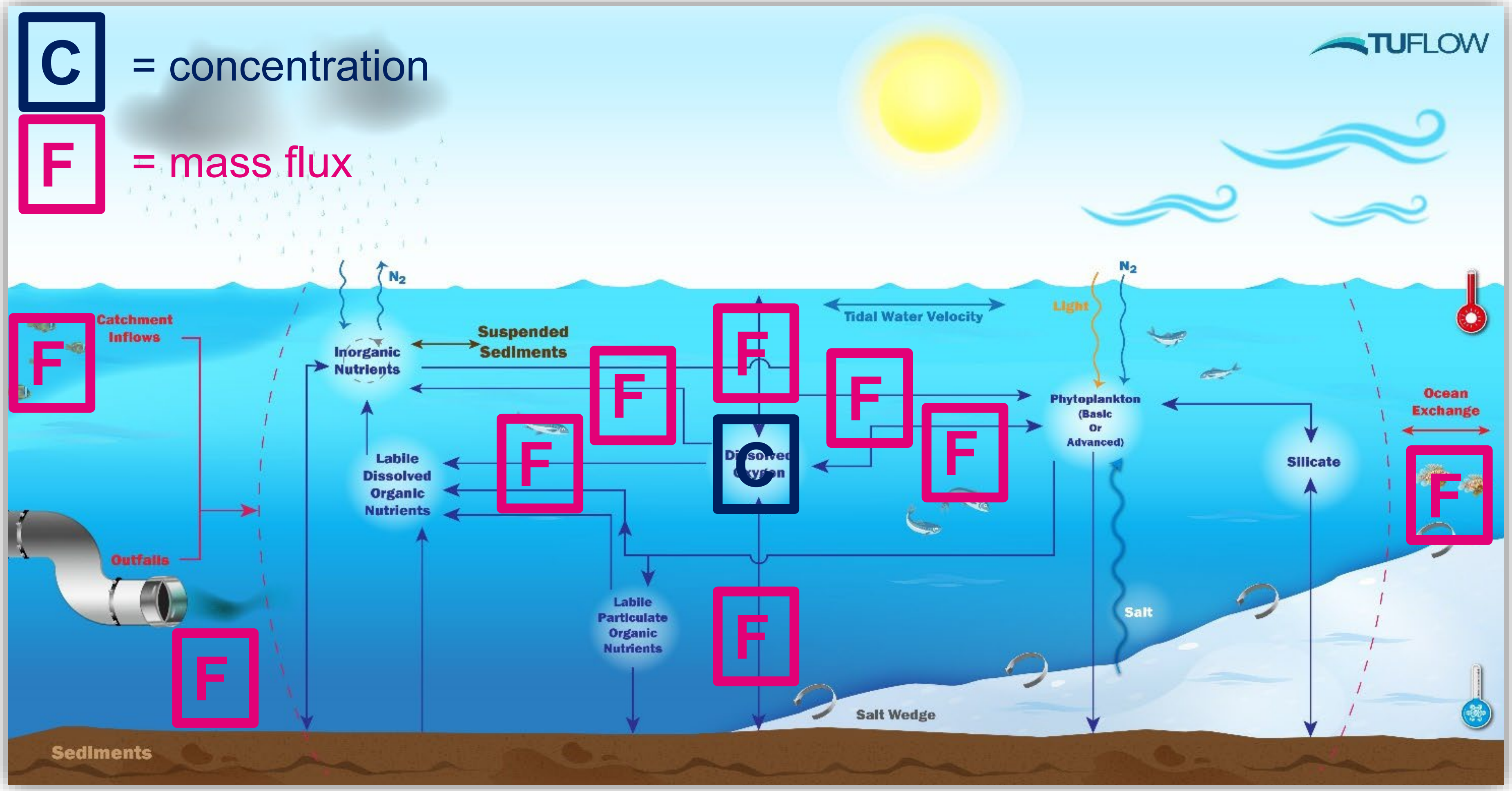
Water quality modelling

- But
  - Dissolved oxygen concentrations are not fundamental quantities: they are the byproduct of multiple environmental oxygen **mass fluxes** (F)
  - Mass fluxes are fundamental quantities

A mass flux is a transfer of mass from one form or state to another

$$CO_2 \longrightarrow C + O_2 \qquad \text{(photosynthesis)}$$

Dissolved oxygen mass fluxes are in milligrams of oxygen per area per day ‘mg/m^2/d’

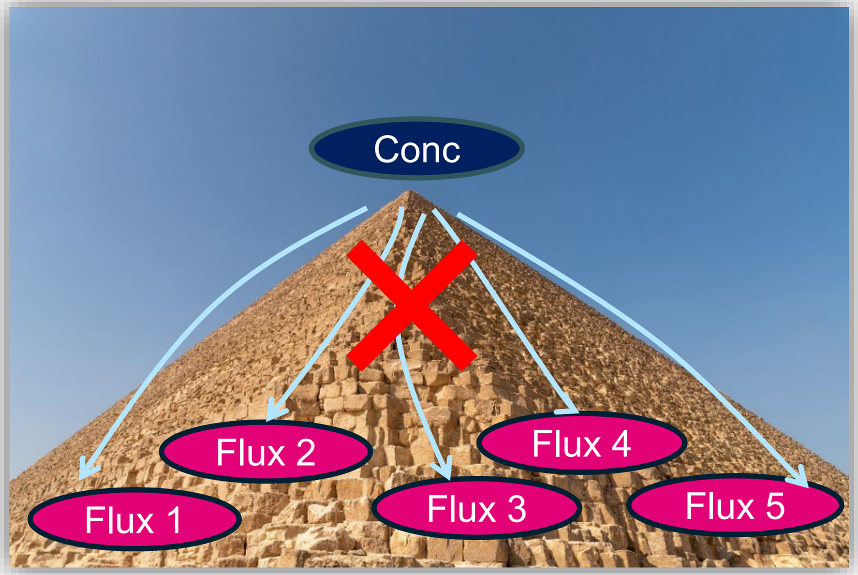

C
= concentration
F
= mass flux
TUFLOW
N2
Catchment Inflows
Inorganic Nutrients
Suspended Sediments
Tidal Water Velocity
Light
N2
Phytoplankton (Basic Or Advanced)
Ocean Exchange
Silicate
Labile Dissolved Organic Nutrients
Dissolved Oxygen
Outfalls
Labile Particulate Organic Nutrients
Salt
Salt Wedge
Sediments

Context

Water quality modelling

- The problem
  - The number 11: is it 6+5 or 20-9?

Concentration → 11; Fluxes → 6, 5



  - A modelled concentration of 11 might match measurements, but is it matching for the right (mass flux) reasons?
  - We cannot tell by looking at a concentrations
  - (But let's hope everything is OK and just get on with our modelling project)

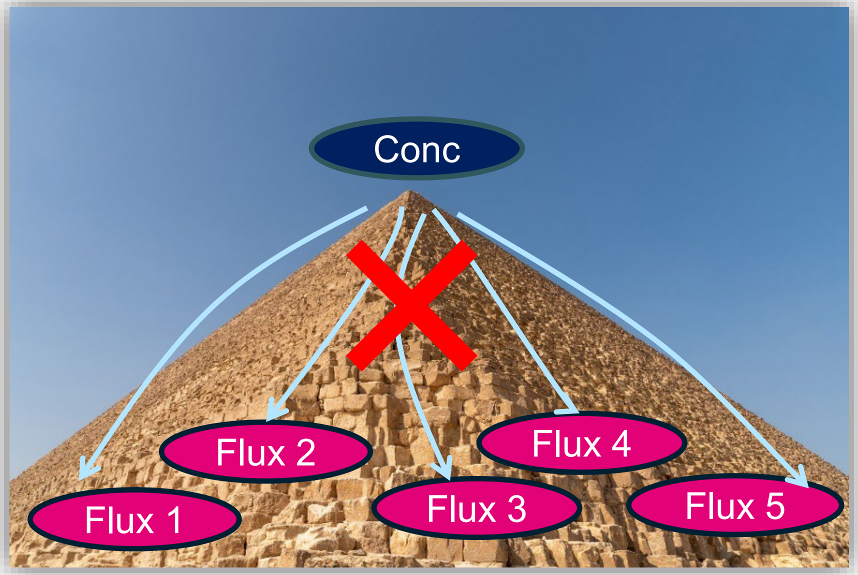
Context

Water quality modelling

- The problem
  - The number 11: is it 6+5 or 20-9?

Concentration — Fluxes

  - A modelled concentration of 11 might match measurements, but is it matching for the right (mass flux) reasons?

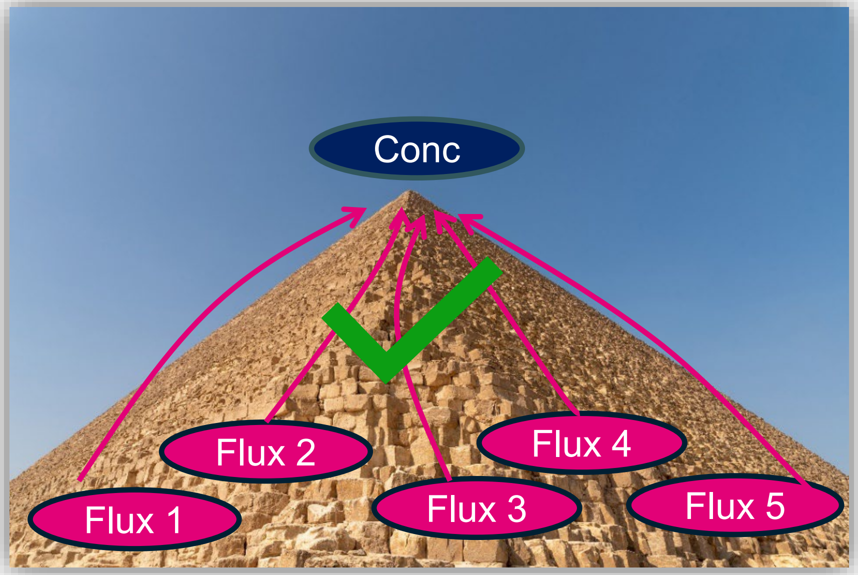


- Standard practise: focus on matching statistics of modelled and measured concentrations

Context

Water quality modelling

- Concentrations == compliance
- Mass fluxes == understanding
- Understanding is needed to develop robust water quality models
- Therefore mass fluxes are an essential part of water quality modelling projects
  - Set up and calibration
  - Peer review and scenarios and predictive power



→ Illustrate through a hypothetical example

The hypothetical

The hypothetical

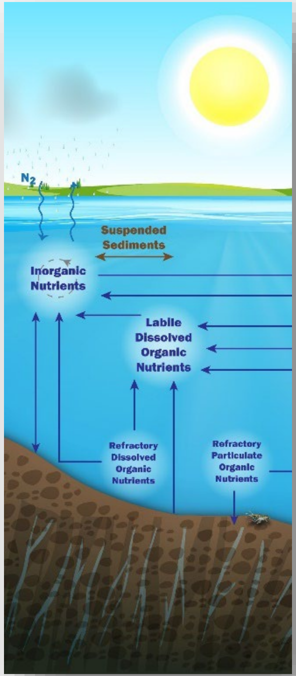
The premise

- A 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
- Real data sets (e.g. bathymetry, rainfall and meteorology) have been used
- Is the model “right” or “fit for purpose” for oxygen simulation?

The hypothetical

The system

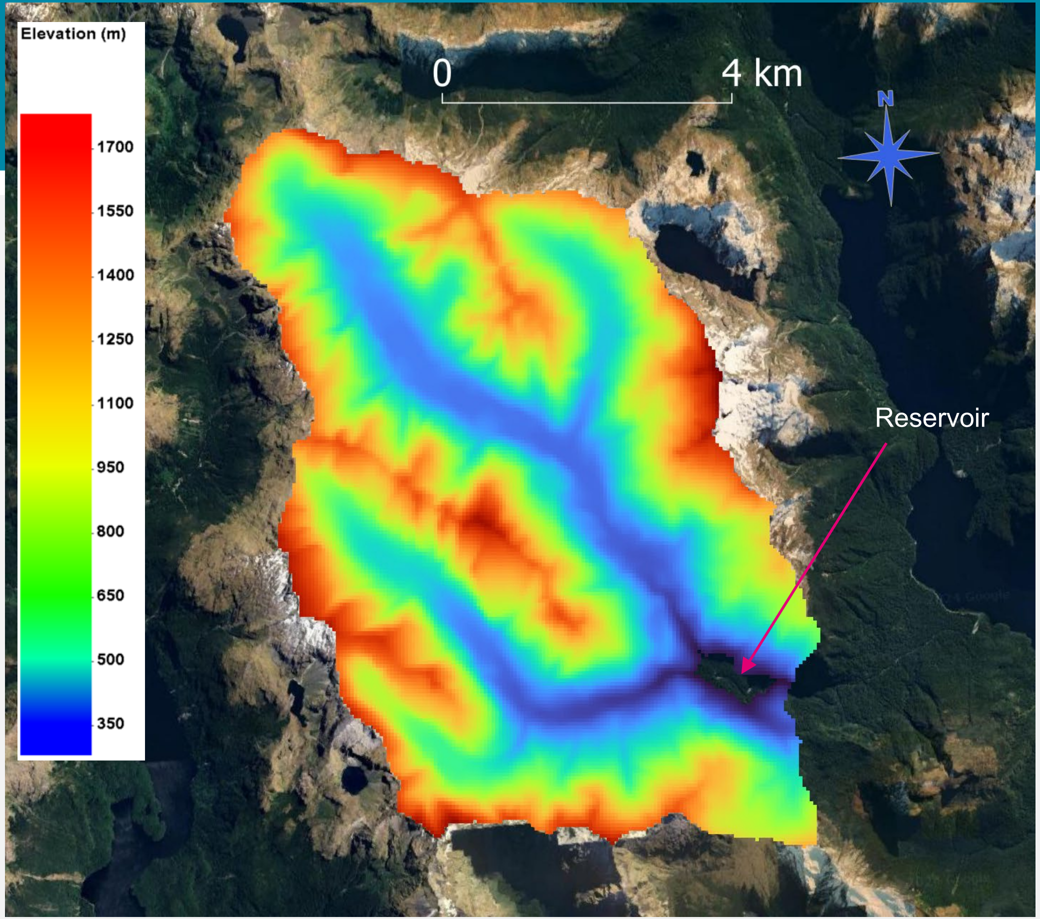
- Catchment
  - 5473 hectares
  - 2534, 2397 and 542 ha forest, agriculture and urban
  - ~700mm annual rainfall
- Reservoir
  - 200 hectare surface area
  - Maximum depth ~35m
  - One offtake and two legacy point source discharges



The hypothetical

The system

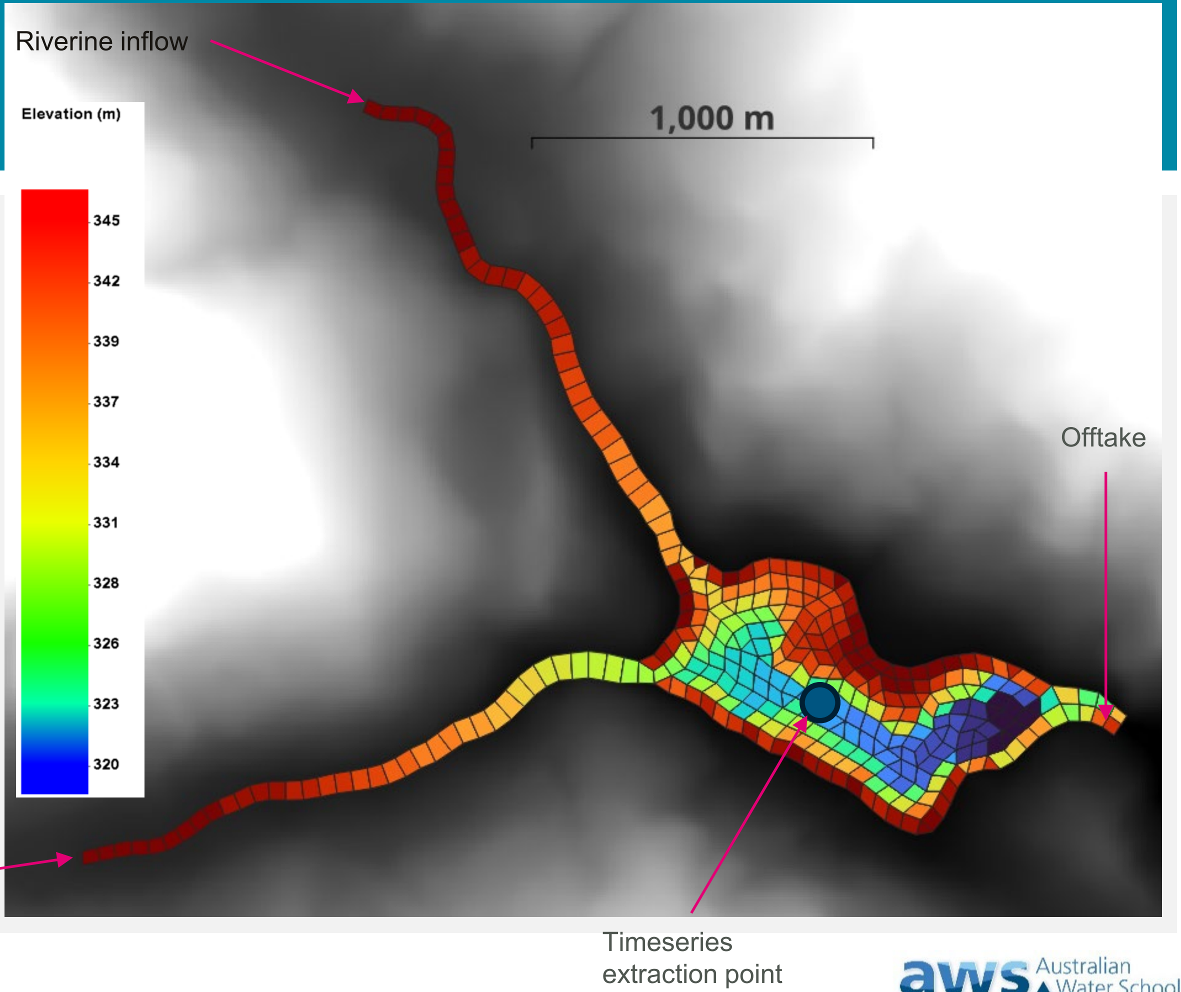
- Catchment
  - 5473 hectares total
  - 2534 ha forest
  - 2397 ha agriculture
  - 542 ha urban
  - ~700mm annual rainfall



The hypothetical

The system

- Reservoir
  - 200 hectares
  - Maximum depth ~35m
  - One offtake and two legacy point source discharges
  - High organic content
  - Coarse resolution



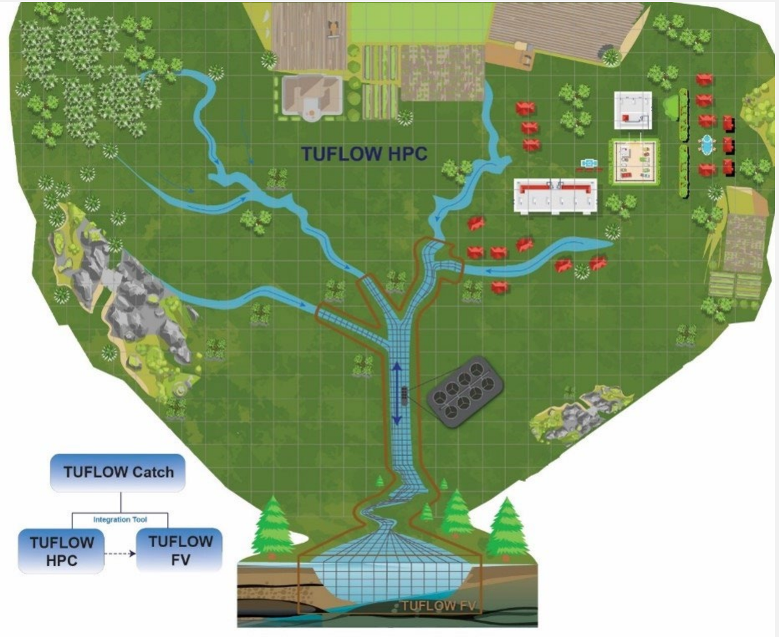
TUFLOW

aws Australian Water School

The hypothetical

The system

- Build a system model
  to assist management
- TUFLOW Catch
  - TUFLOW HPC Catchment hydrology
    and pollutant export
  - TUFLOW FV in-lake 3D water quality
- See our previous TUFLOW water quality
  webinar!



- https://awschool.com.au/training/webinar-integrated-catchment-and-receiving-water-modelling/

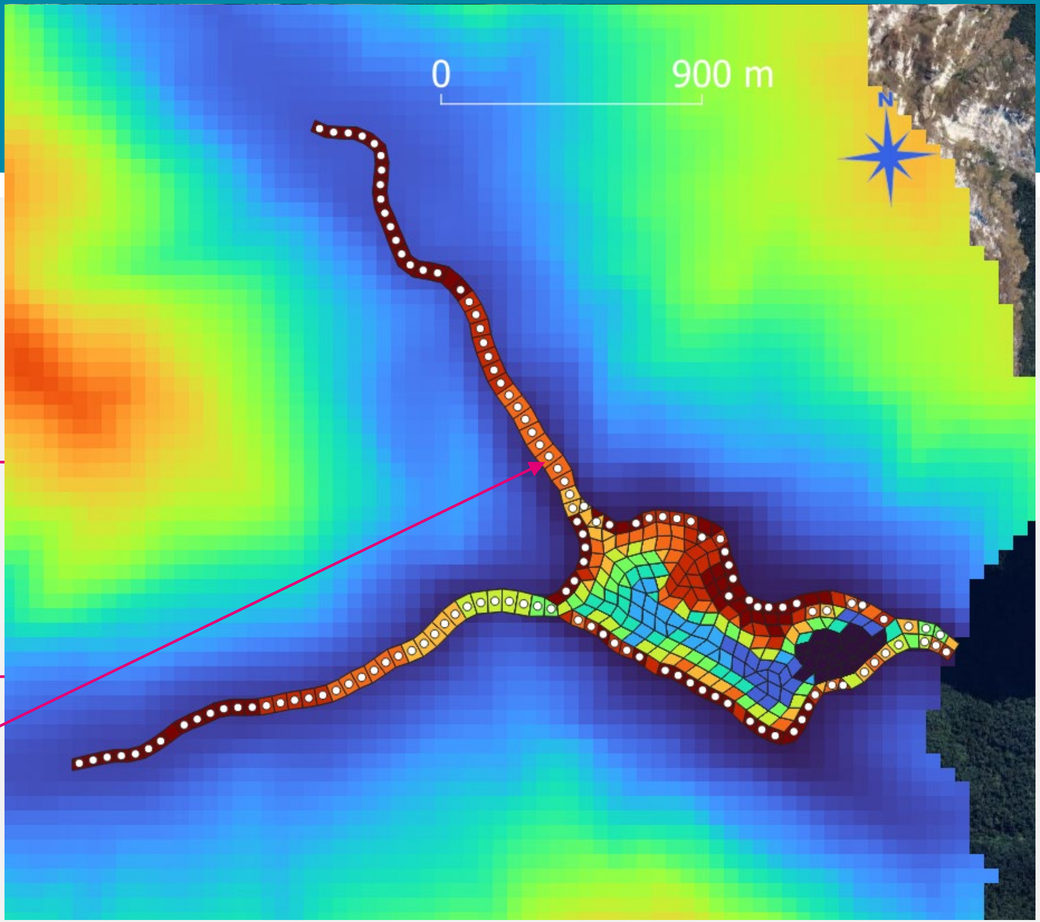
The hypothetical

The model

TUFLOW HPC Domain

TUFLOW FV Domain

Automatically determined connection boundary points (white dots)



Dissolved oxygen

The hypothetical

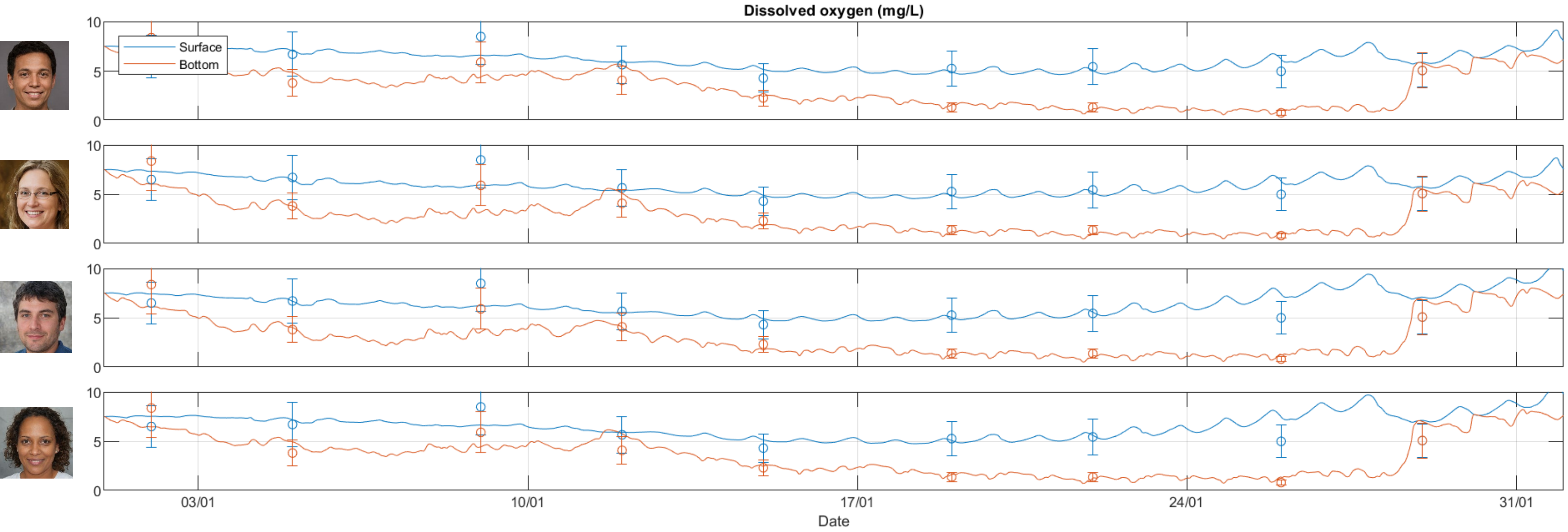
Dissolved oxygen

- Prediction / “calibration” to concentrations
- Four modellers
  - Ray
  - Phyllis
  - Ron
  - Brenda
- I am the peer reviewer




The hypothetical

Dissolved oxygen concentration timeseries



The hypothetical

Dissolved oxygen

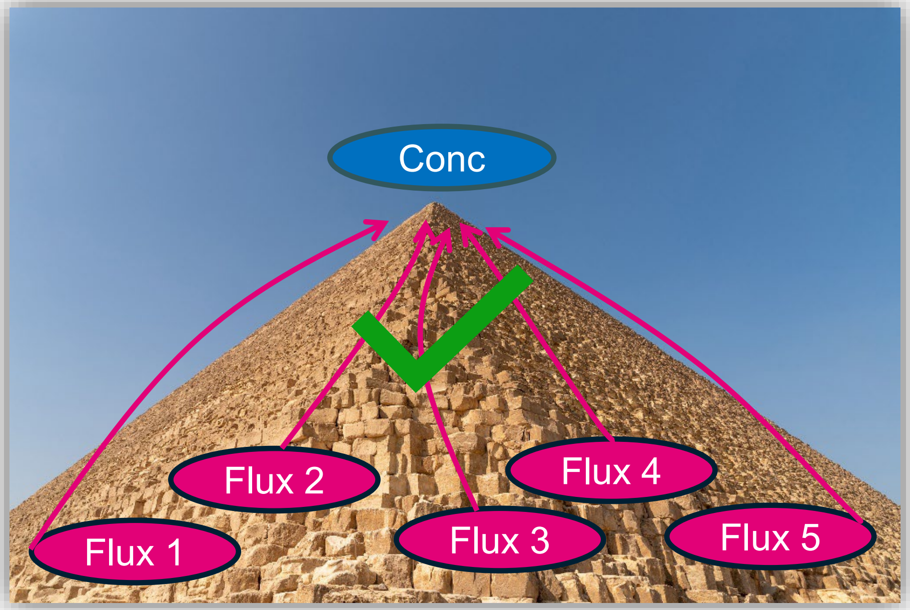
- Prediction / “calibration” to concentrations
- Moriasi 2015
  - Very good
  - Good
  - Satisfactory
  - Not satisfactory

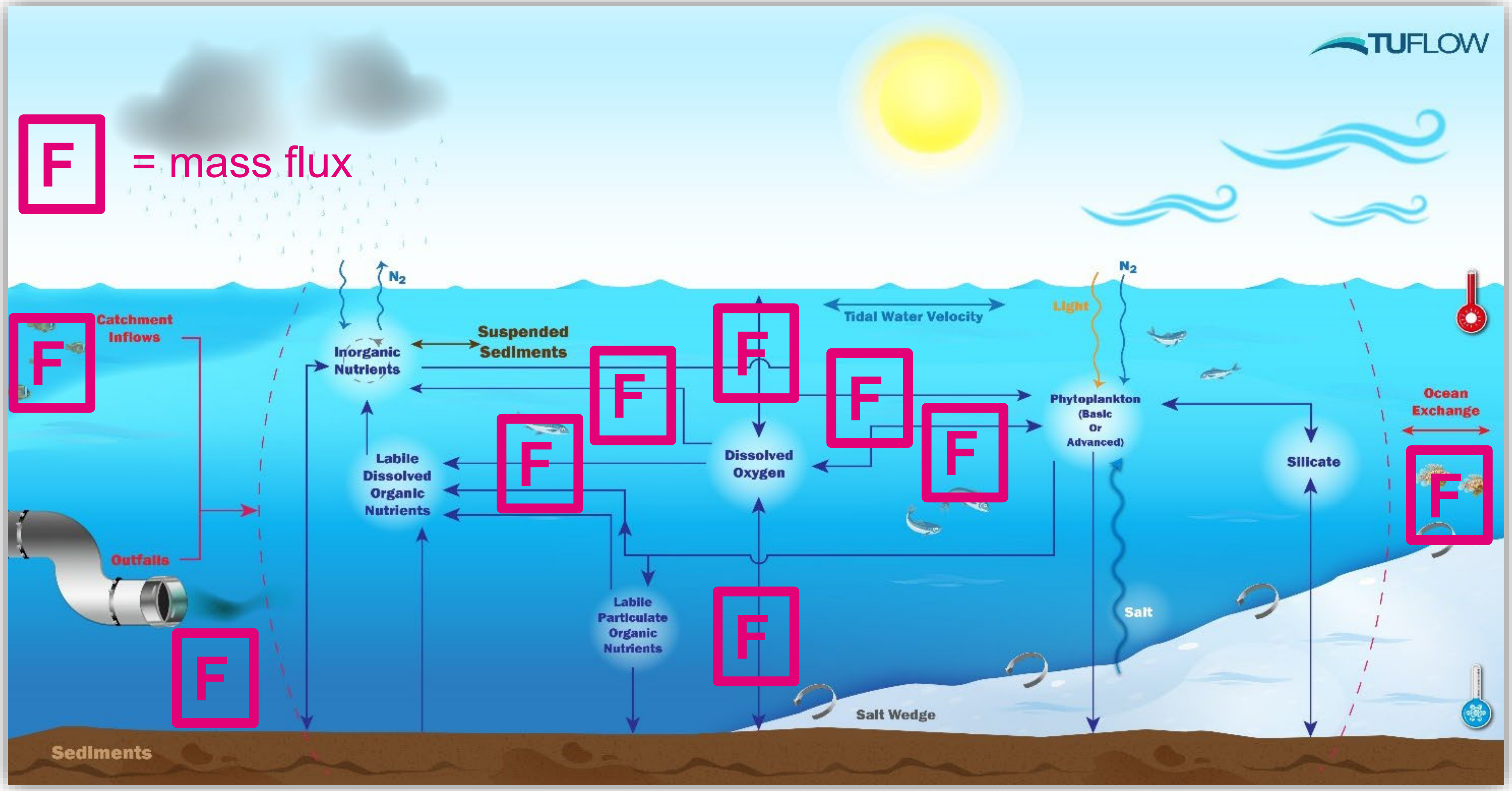
Metric	Ray	Phyllis	Ron	Brenda
R	0.89	0.85	0.81	0.83
R^2	0.79	0.72	0.66	0.69
NSE	0.78	0.70	0.63	0.65
IOA	0.93	0.91	0.90	0.90
RMSE	1.0	1.2	1.3	1.3
MAE	0.8	0.8	0.9	1.0
PBIAS	-2.8	5.4	-0.4	-8.8

The hypothetical

Dissolved oxygen

- But how do 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 mass fluxes!



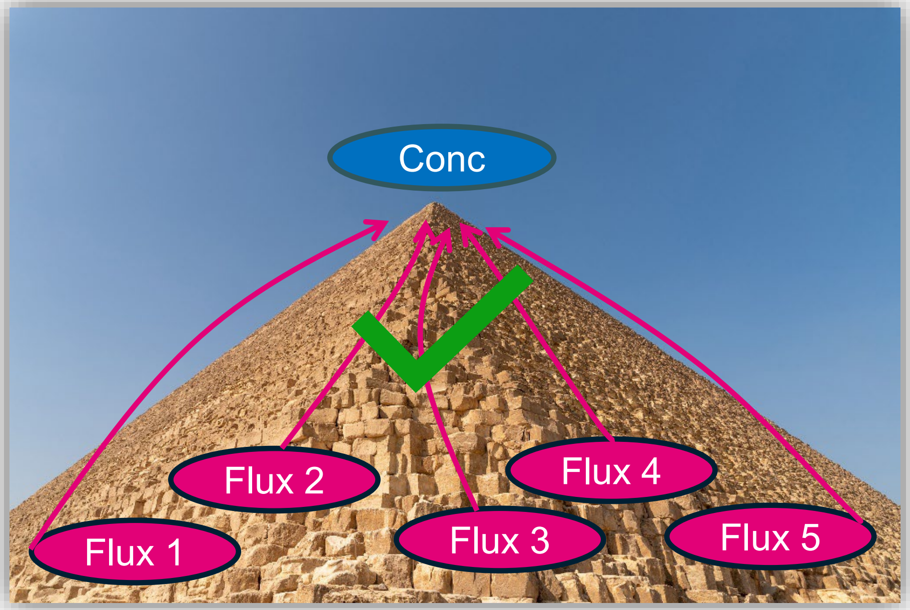


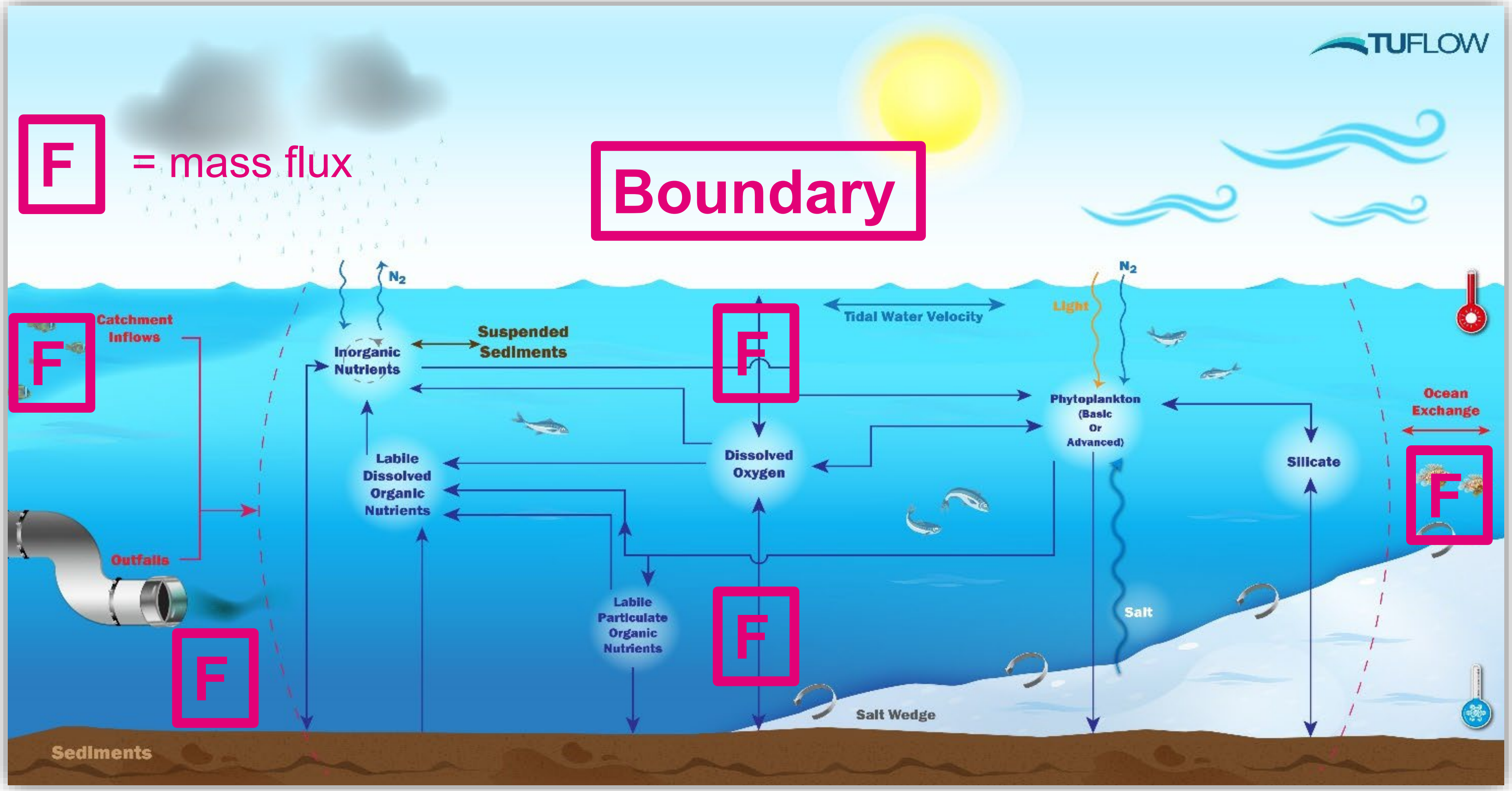
F = mass flux
N2
Catchment Inflows
Outfalls
Inorganic Nutrients
Suspended Sediments
Tidal Water Velocity
Light
N2
Phytoplankton (Basic Or Advanced)
Ocean Exchange
Silicate
Dissolved Oxygen
Labile Dissolved Organic Nutrients
Labile Particulate Organic Nutrients
Salt
Salt Wedge
Sediments
F
F
F
F
F
F
F
F
F
F

The hypothetical

Dissolved oxygen

- Boundary oxygen fluxes
  - Sediments: consume
  - Surface aeration: produce / consume
  - Catchments: produce
  - WWTPs: produce
  - Offtake: consume





F
= mass flux
Boundary
Catchment Inflows
Outfalls
Inorganic Nutrients
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Light
Phytoplankton (Basic Or Advanced)
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Labile Dissolved Organic Nutrients
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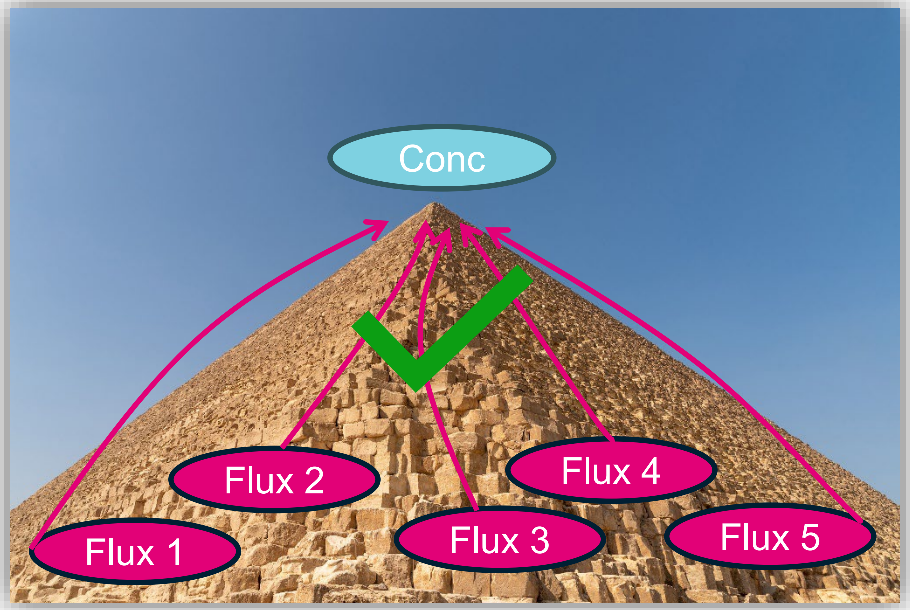
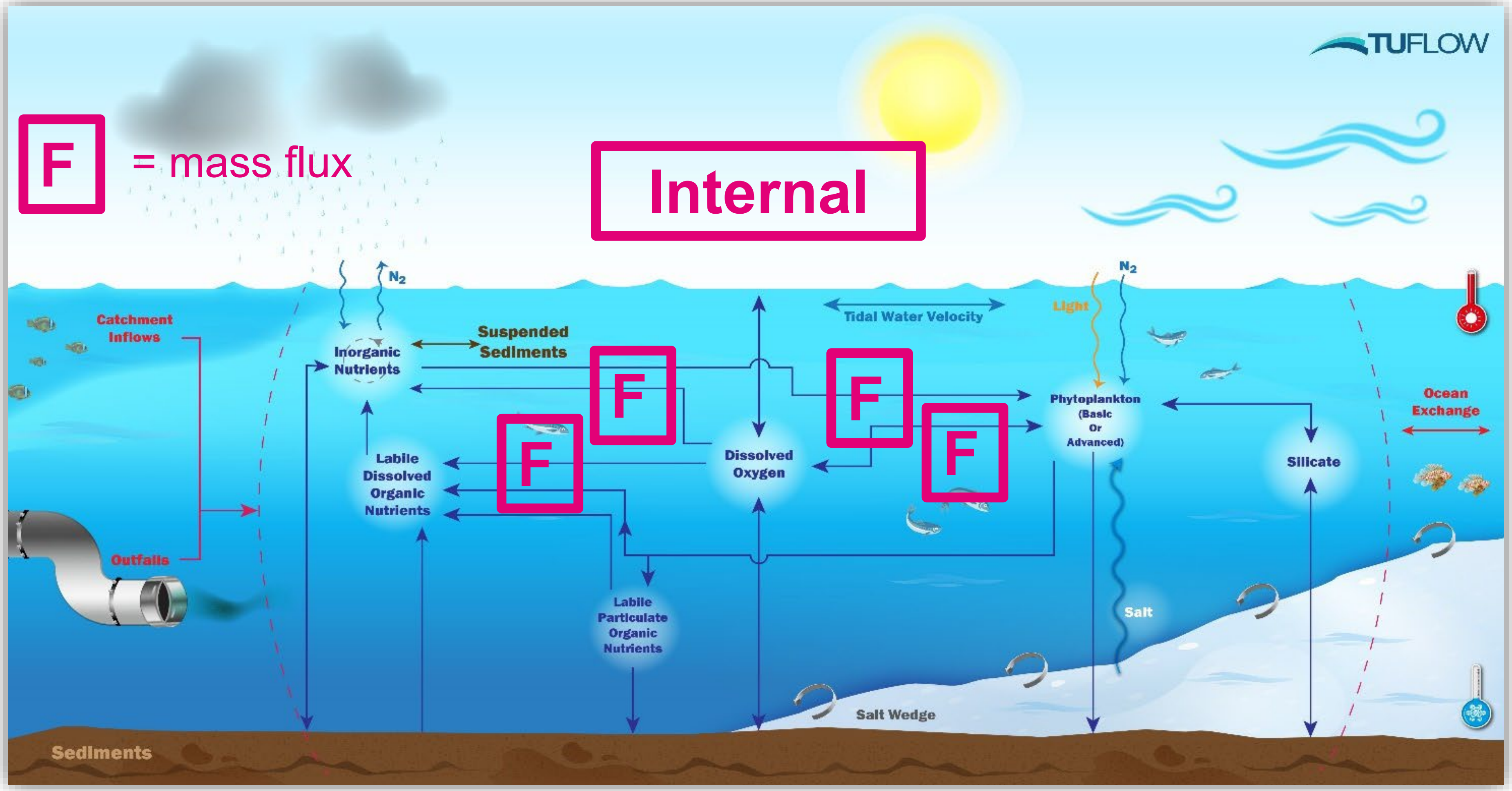
TUFLOW

The hypothetical

Dissolved oxygen

- Internal oxygen fluxes
  - Phytoplankton respiration: consume
  - Organic matter mineralisation: consume
  - Ammonium nitrification: consume
  - Phytoplankton primary productivity: produce





F
= mass flux
Internal
Catchment Inflows
Outfalls
N_2
Inorganic Nutrients
Suspended Sediments
Tidal Water Velocity
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N_2
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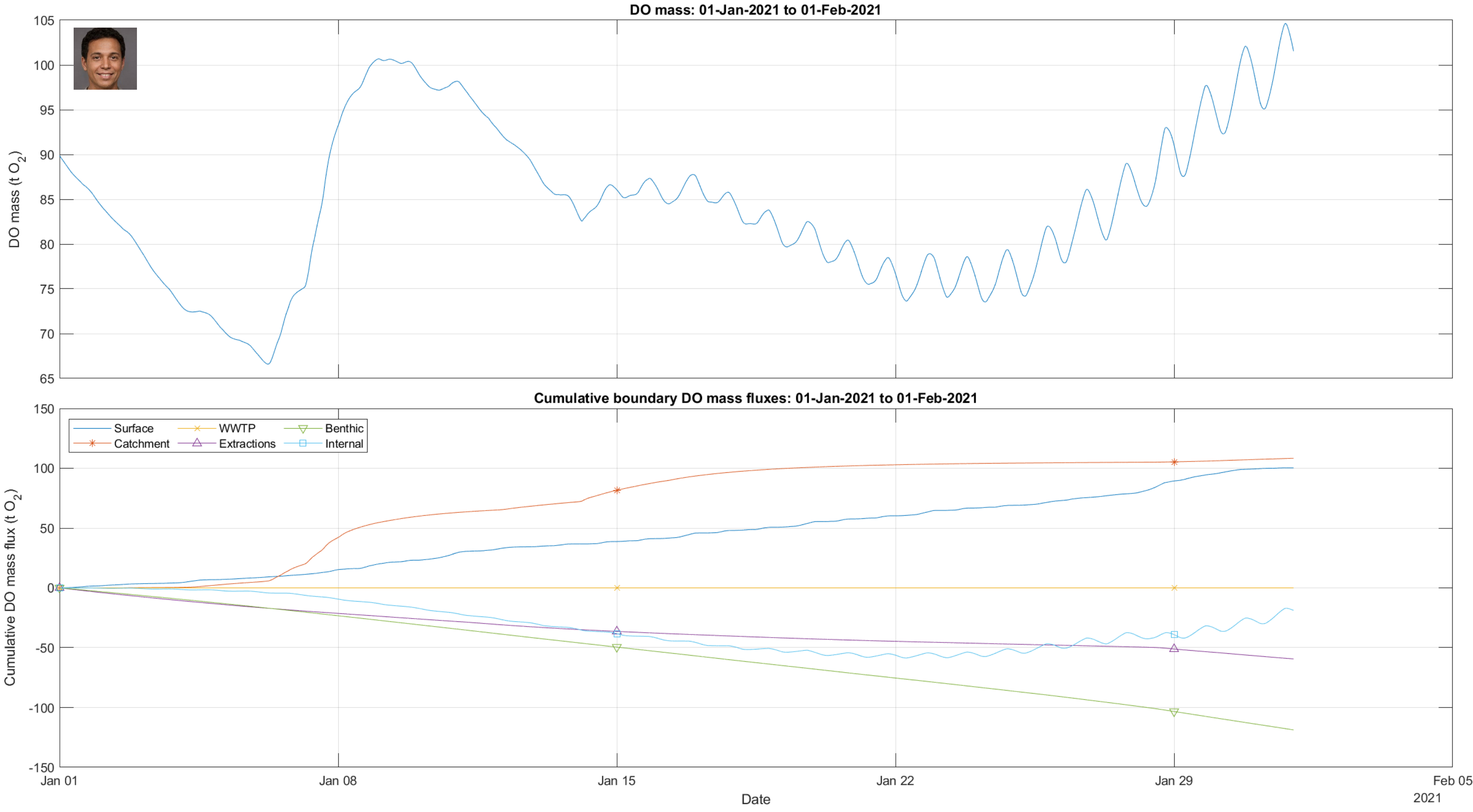
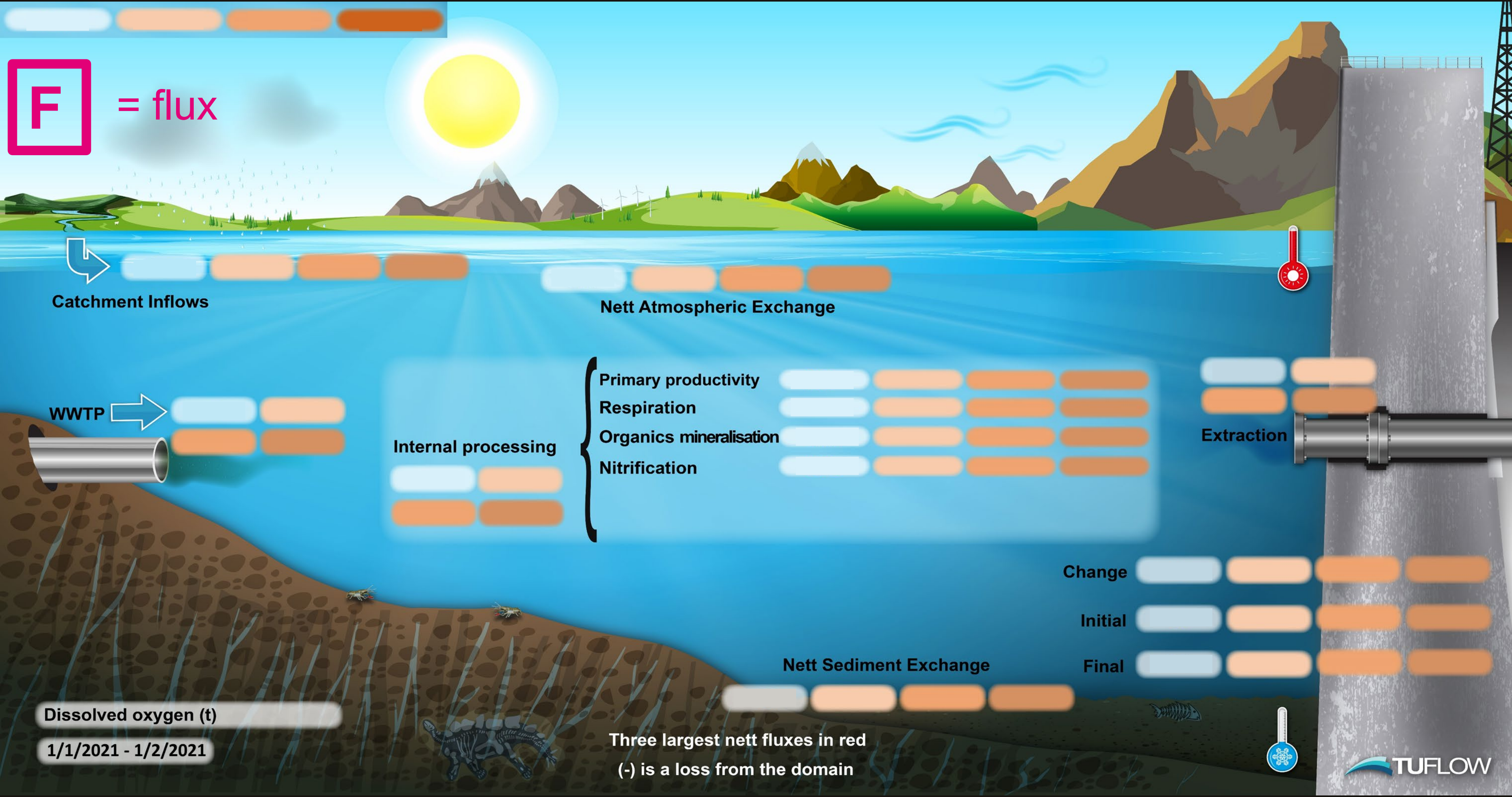
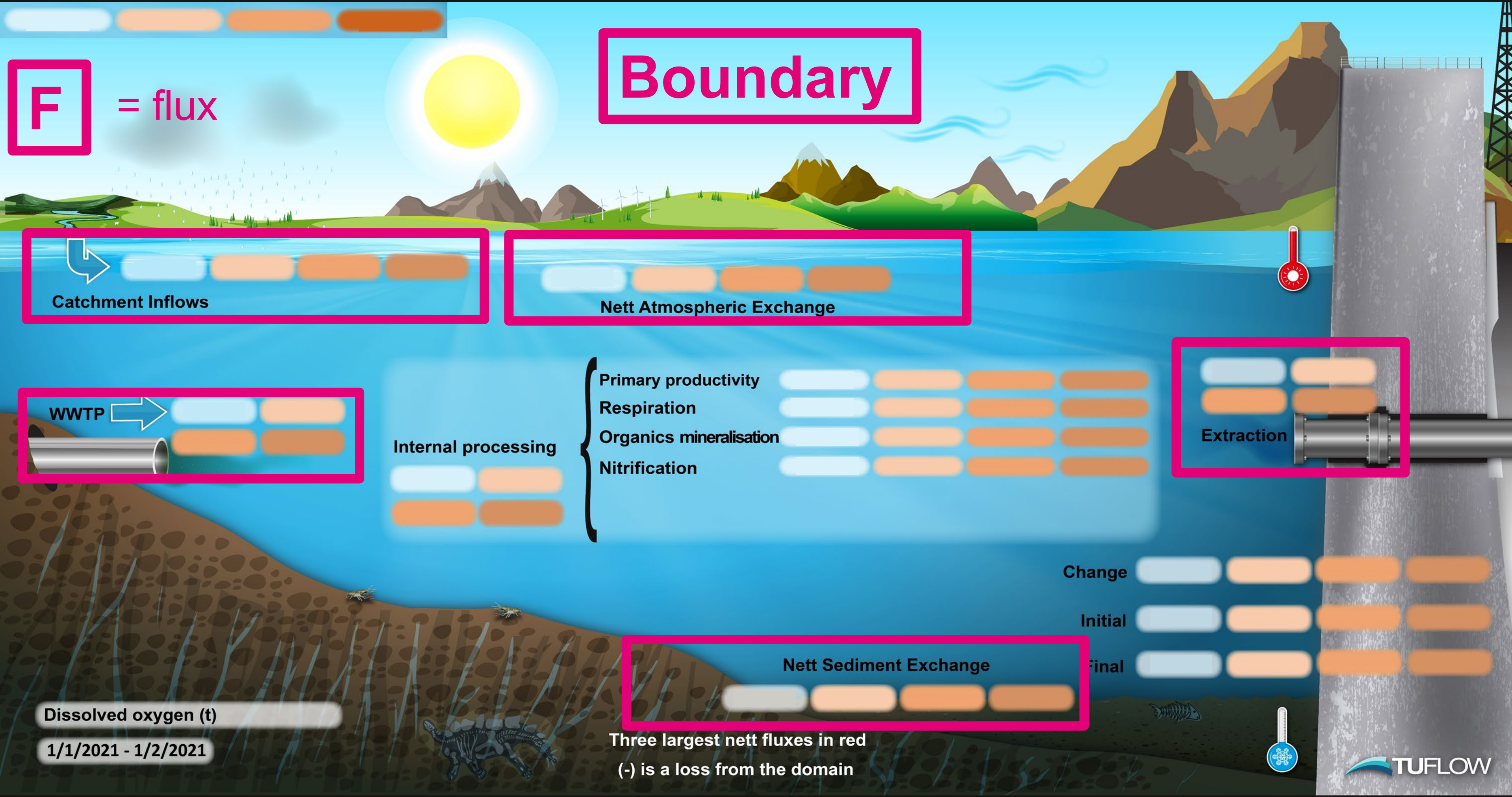
TUFLOW


DO mass: 01-Jan-2021 to 01-Feb-2021
DO mass (t O2)
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 O2)
150
100
50
0
-50
-100
-150
Jan 01
Jan 08
Jan 15
Jan 22
Jan 29
Feb 05
2021
Date



F = flux
Catchment Inflows
Nett Atmospheric Exchange
WWTP
Internal processing
Primary productivity
Respiration
Organics mineralisation
Nitrification
Extraction
Change
Initial
Final
Nett Sediment Exchange
Dissolved oxygen (t)
1/1/2021 - 1/2/2021
Three largest nett fluxes in red
(-) is a loss from the domain
TUFLOW



Boundary
F = flux
Catchment Inflows
Nett Atmospheric Exchange
WWTP
Internal processing
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Initial
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Dissolved oxygen (t)
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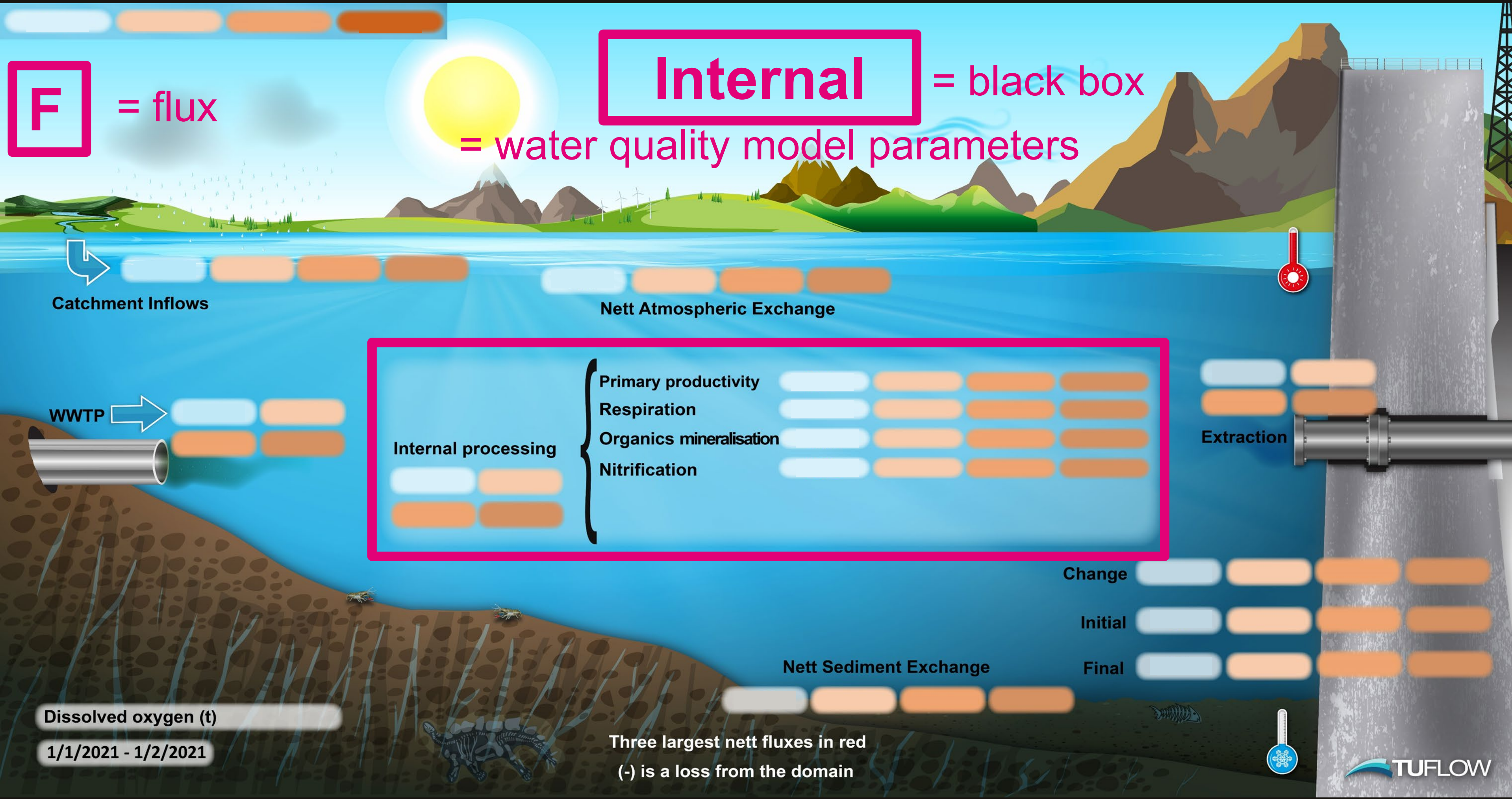

F
= flux
Internal
= black box
= water quality model parameters
Catchment Inflows
Nett Atmospheric Exchange
WWTP
Internal processing
Primary productivity
Respiration
Organics mineralisation
Nitrification
Extraction
Change
Initial
Final
Nett Sediment Exchange
Dissolved oxygen (t)
1/1/2021 - 1/2/2021
Three largest nett fluxes in red
(-) is a loss from the domain
TUFLOW

Ray
F
= flux
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


Ray
Phyllis
F = flux
108
108
Catchment Inflows
100
113
Nett Atmospheric Exchange
WWTP
0
0
Internal processing
-19
-5
Primary productivity
276
284
Respiration
-30
Organics mineralisation
-135
-222
Nitrification
-131
-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

Ray
Phyllis
Ron
F
= flux
108
108
108
Catchment Inflows
100
113
85
Nett Atmospheric Exchange
WWTP
0
0
0
Internal processing
-19
-5
52
Primary productivity
Respiration
Organics mineralisation
Nitrification
276
284
300
-30
-135
-222
-131
-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

Ray
Phyllis
Ron
Brenda
F = flux
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 -28
Organics mineralisation -135 -222 -148
Nitrification -131 -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
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TUFLOW

The hypothetical

Dissolved oxygen

- Prediction / “calibration” to concentrations
- Moriasi 2015
  - Very good
  - Good
  - Satisfactory
  - Not satisfactory

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The outcome

Dissolved oxygen

- Solutions
  - Our modellers have the right answers for the wrong reasons!
  - Predictive capability is therefore compromised as the underlying processes are incorrect
- So what do we do?

The outcome

Dissolved oxygen

- Engage and understand via flux diagnostics discussion to understand
  - Report and analyse fluxes
  - Managers and decision makers
  - Traditional owners
  - Local knowledge
  - …non-modellers!

The outcome

Dissolved oxygen

- Fluxes can be measured (but aren’t as often!)
  - Sediment
  - Phytoplankton
  - Organics
  - Inorganics

The wrap

The wrap

Concentrations and fluxes

- Not new
  - Hipsey et al. (2020)
  - Same for all constituents, not just oxygen

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]

The wrap

Concentrations and fluxes

- Comparing model concentration timeseries with point field measurements (or medians, or by zones) actively excludes understanding
  - Wasteful calibration time – often the major project and community resource sink
  - End up arguing over modelled timeseries and measured points not matching
  - Wasteful scenarios
- So
  - Measure fluxes more routinely
  - Use numerical modelling tools that report mass fluxes, e.g. TUFLOW FV WQ module

Questions?