Comparison of WRTDS and GAMs for evaluating long-term trends in chlorophyll

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Since the last call...

- Application of GAMs and WRTDS to 30 year time series of monthly chlorophyll at LE1.2 and TF1.6
- Development of comparable methods for model fitting
- Development of simulated datasets to evaluate flow-normalization
- Comparison of results and conclusions

Model applications

Both models used vertically-integrated chlorophyll, monthly timestep

LE1.2: lnchla $\sim$ time + ***salinity***

TF1.6: lnchla $\sim$ time + ***flow***

Fits evaluated for whole time series and annual/seasonal/flow aggregations:

- predicted to observed, GAM predicted to WRTDS predicted
- Trends in flow-normalized results (average and % change overall, by time period)

Model comparisons of flow-normalized results with simulated datasets

Model applications

For comparing each model's ***predictions to observed***, at both sites:

$$RMSE_{fit} = \sqrt{\frac{\sum_{i=1}^{n}\left(Chl_i - \widehat{Chl}_i\right)^2}{n}}$$

For comparing ***predictions between models***, at both sites:

$$RMSE_{btw} = \sqrt{\frac{\sum_{i=1}^{n}\left(\widehat{Chl}_{WRTDS,\,i} - \widehat{Chl}_{GAM,\,i}\right)^2}{n}}$$

$$\text{Average difference} = \left(\frac{\sum_{i=1}^{n}\widehat{Chl}_{WRTDS,\,i} - \sum_{i=1}^{n}\widehat{Chl}_{GAM,\,i}}{\sum_{i=1}^{n}\widehat{Chl}_{GAM,\,i}}\right) * 100$$

Development of comparable methods

Objective: Compare models on the same playing field

Problem: Need methods to prevent over-fitting for comparability

GAMs: identify optimal smoothing parameter to balance fit and 'wiggliness'

WRTDS: identify optimal window widths for time, discharge (salinity or flow), and season

Existing method for GAMs, k-fold cross-validation and search algorithm ('limited memory BFGS quasi-Newton method') to identify window-widths for WRTDS

Development of simulated datasets

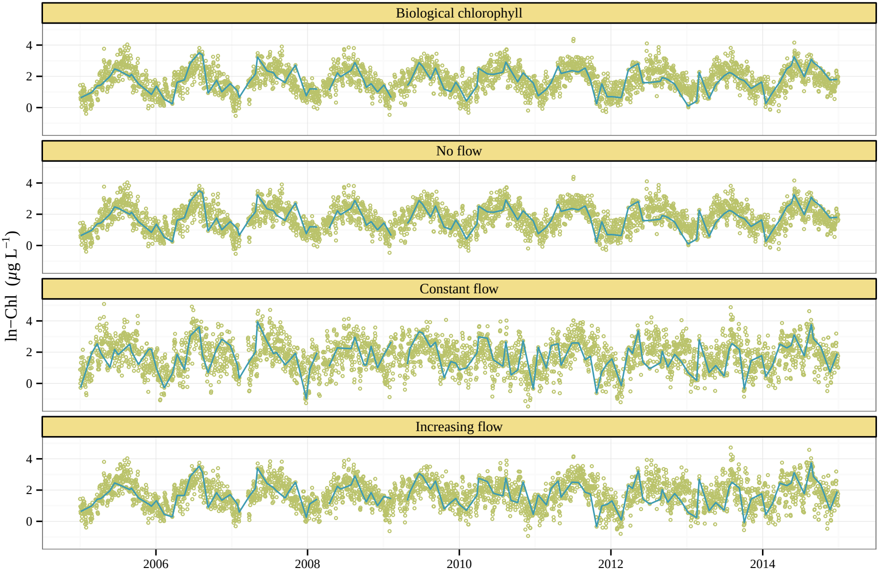
Objective: Evaluate ability of each model to reproduce flow-normalized trends

Problem: The true flow-normalized trends are not known and can only be empirically estimated

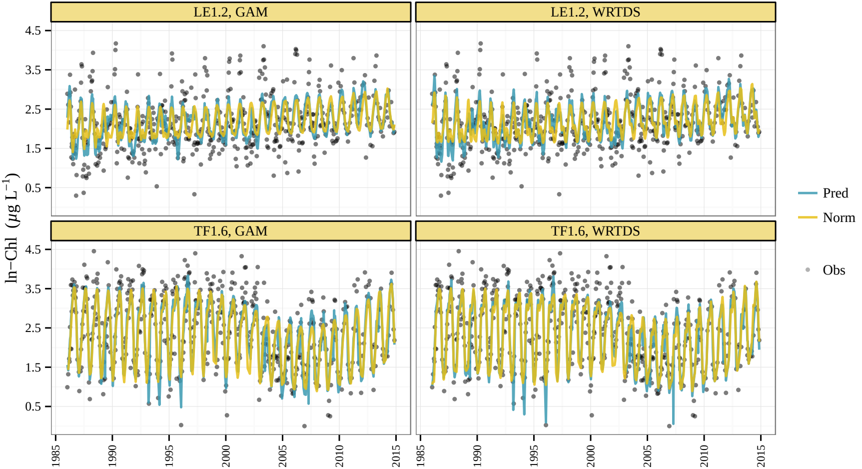
We simulated monthly datasets following techniques in Beck et al. 2015 and Hirsch et al. 2015

- Daily time series: Bowie gage discharge, Jug Bay fluorescence
- Overall: $Chl_{obs} = Chl_{flo} + Chl_{bio}$
- From discharge: $Chl_{flo} = I\left(\widehat{Q}_{seas} + \sigma \cdot \varepsilon_{Q,\,sim}\right)$
- From fluorescence: $Chl_{bio} = \widehat{Chl}_{seas} + \sigma \cdot \varepsilon_{Chl,\,sim}$
- Indicator I changes to simulate changing flow component

Development of simulated datasets

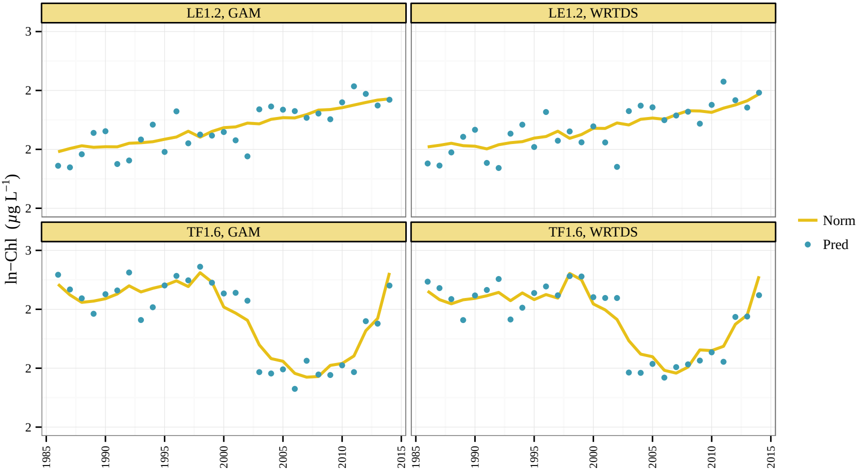


Results



LE1.2, GAM
LE1.2, WRTDS
TF1.6, GAM
TF1.6, WRTDS
ln−Chl (μg L−1)
4.5
3.5
2.5
1.5
0.5
1985
1990
1995
2000
2005
2010
2015
Pred
Norm
Obs

Results



LE1.2, GAM
LE1.2, WRTDS
TF1.6, GAM
TF1.6, WRTDS
ln−Chl (μg L^{-1})
3
2
2
2
1985
1990
1995
2000
2005
2010
2015
Norm
Pred

Results

Table : RMSE of observed to predicted ln-chlorophyll.

Period	**LE1.2**		**TF1.6**	
	GAM	WRTDS	GAM	WRTDS
All				
	0.54	0.51	0.54	0.52
Annual				
1986-1993	0.54	0.50	0.53	0.49
1994-2000	0.52	0.50	0.58	0.58
2001-2007	0.63	0.60	0.54	0.53
2008-2014	0.39	0.36	0.49	0.44
Seasonal				
JFM	0.61	0.58	0.53	0.49
AMJ	0.69	0.64	0.60	0.58
JAS	0.38	0.35	0.48	0.46
OND	0.41	0.38	0.55	0.54
Flow				
1 (Low)	0.40	0.36	0.48	0.46
2	0.47	0.42	0.56	0.54
3	0.61	0.57	0.56	0.52
4 (High)	0.64	0.63	0.56	0.54

Results

Table : Comparison of predicted results between models.

Period	LE1.2		TF1.6	
	Ave. diff.	RMSE	Ave. diff.	RMSE
All				
	-0.11	0.15	0.01	0.17
Annual				
1986-1993	0.18	0.16	-0.78	0.17
1994-2000	0.53	0.15	-1.09	0.19
2001-2007	-0.95	0.14	0.48	0.14
2008-2014	-0.18	0.14	3.12	0.18
Seasonal				
JFM	2.91	0.14	-5.02	0.22
AMJ	-3.42	0.17	0.93	0.14
JAS	5.03	0.14	-0.10	0.17
OND	-5.25	0.14	2.08	0.17
Flow				
Flow 1 (Low)	0.19	0.16	-0.09	0.12
Flow 2	-0.83	0.16	0.73	0.15
Flow 3	0.19	0.15	0.84	0.20
Flow 4 (High)	0.03	0.13	-1.62	0.20

Results

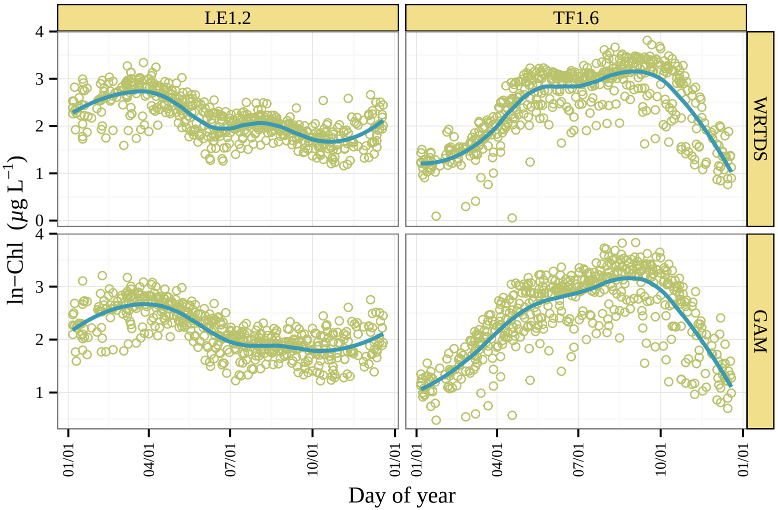


Figure : Seasonal variation from model predictions.

Results

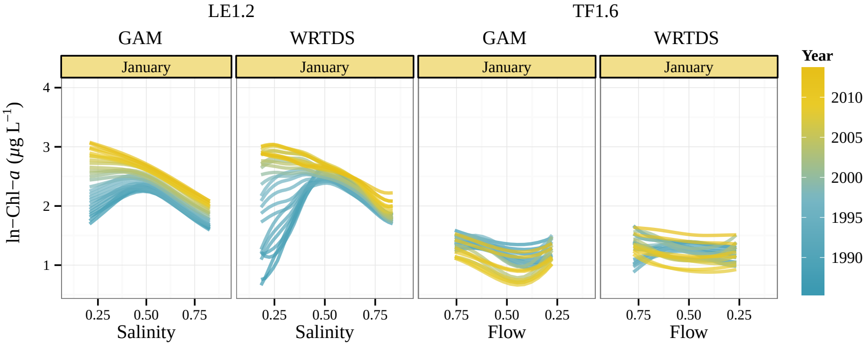
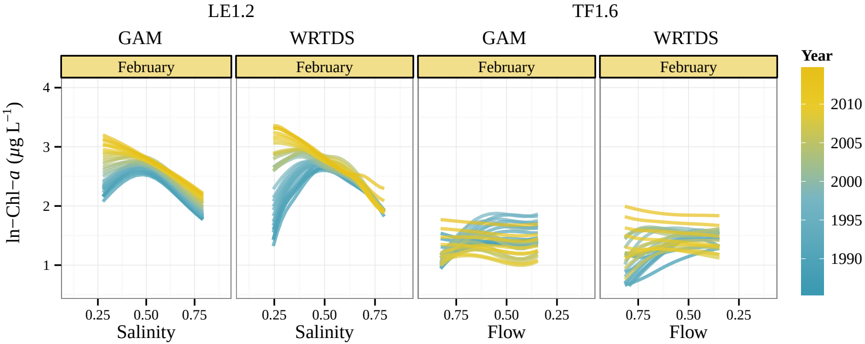


Figure : Changes in the relationship between chlorophyll and flow across the time series with separate plots by month, model, and station. The scales of salinity and flow are reversed for trend comparison with units in proportion of the total range for each month.

Results



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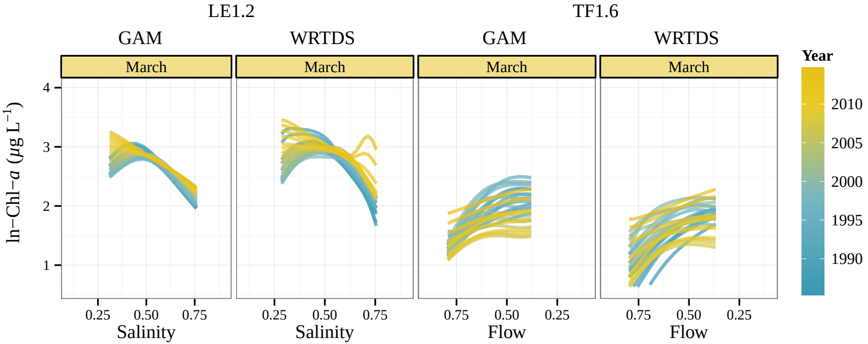

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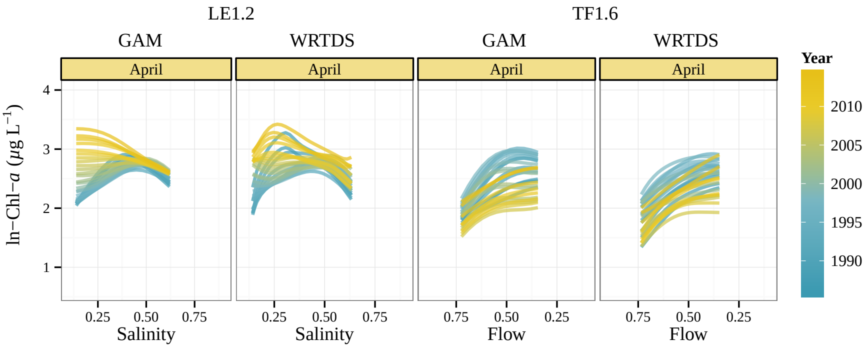

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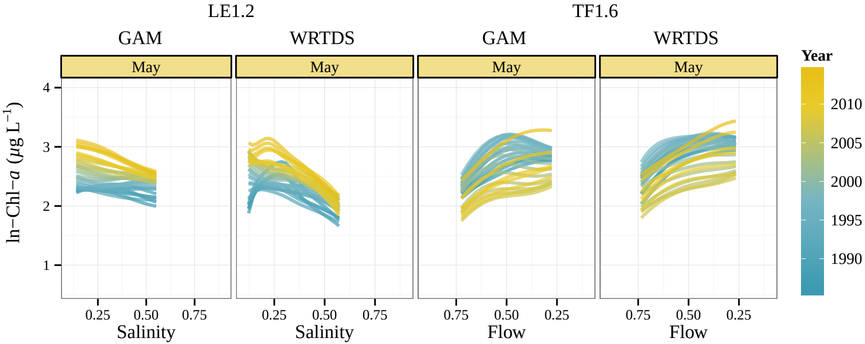

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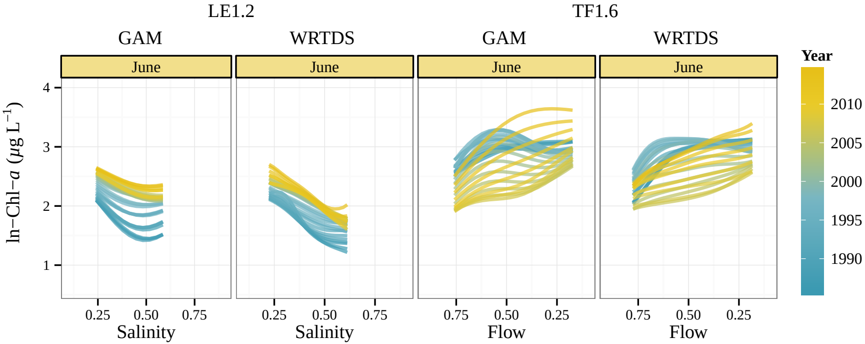

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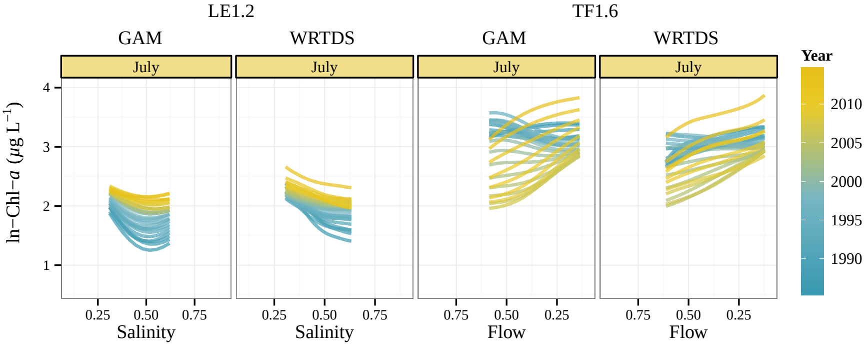

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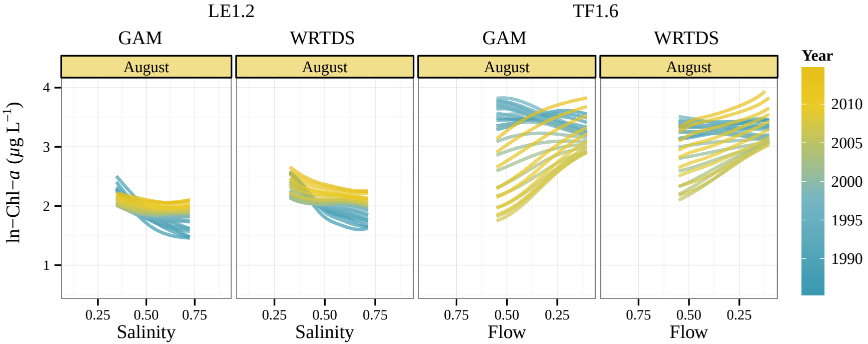

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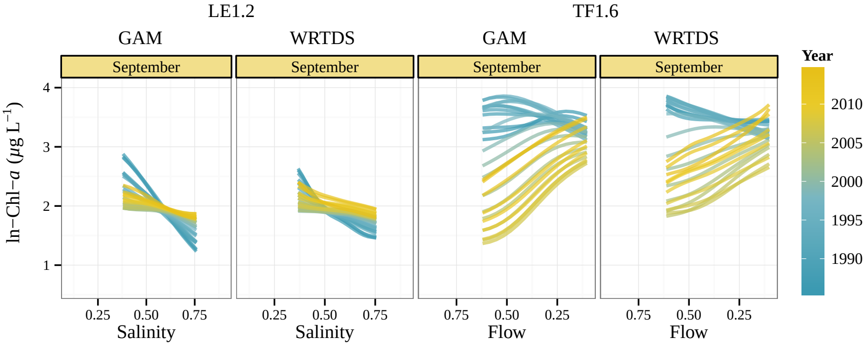

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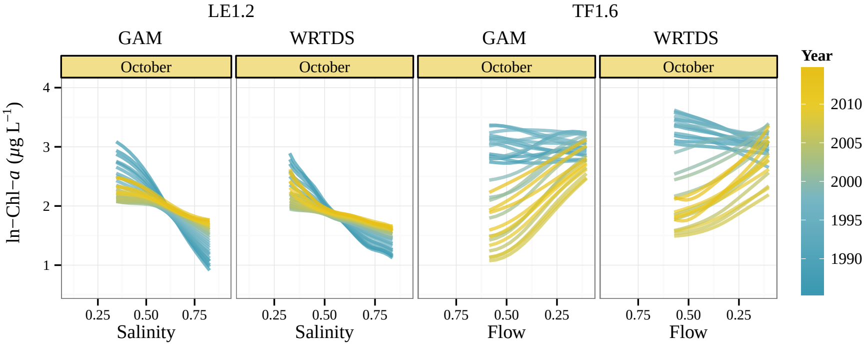

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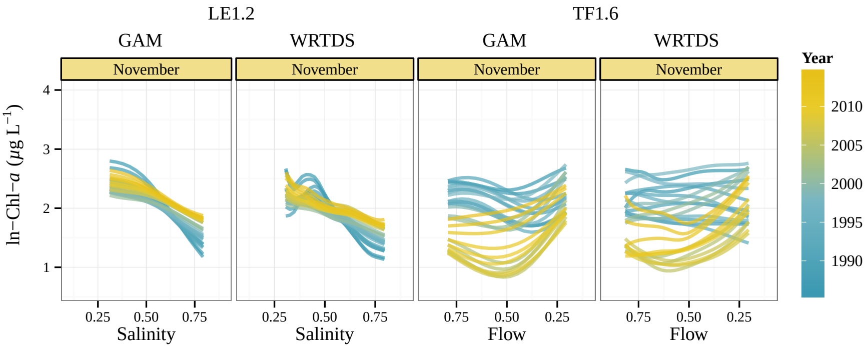

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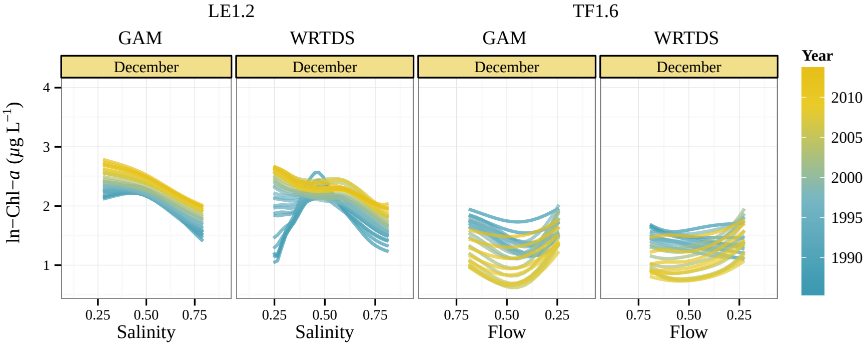

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Results

Simulated data behaved as expected: three datasets with different flow contributions

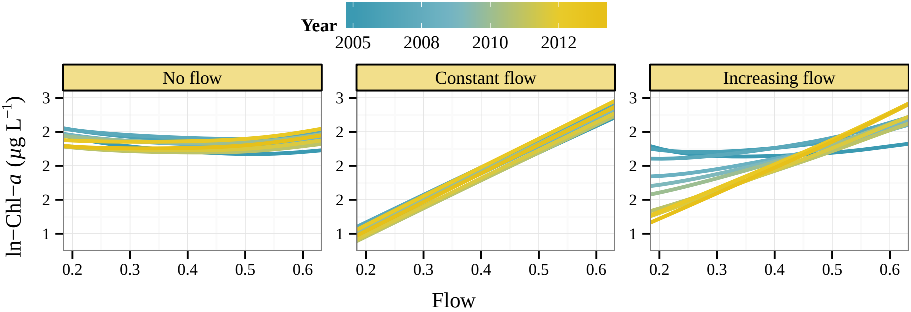

Figure : WRTDS predictions from August for three simulated datasets with different flow contributions.

Results

Objective: How well do flow-normalized predictions for each model reproduce Chl_{flo}

Simulated time series: $Chl_{obs} = Chl_{flo} + Chl_{bio}$

Table : Performance summaries (RMSE) of model predictions for the three simulated time series (no flow, constant flow, and increasing flow effect).

Simulations	$Chl_{obs} \sim \widehat{Chl}_{obs}$	$Chl_{bio} \sim \widehat{Chl}_{bio}$
No flow		
GAM	0.51	0.53
WRTDS	0.50	0.52
Constant flow		
GAM	0.51	0.58
WRTDS	0.53	0.57
Increasing flow		
GAM	0.51	0.54
WRTDS	0.50	0.52

Conclusions

- WRTDS always 'out-performed' GAMs, improvement was minimal
- Seasonal patterns better described by WRTDS
- No clear differences in flow-normalization abilities
- Interesting trends in Patuxent
  - Chlorophyll increasing lower estuary (LE1.2), mainstem influences
  - Multi-year signal of Isabel at TF1.6, flushing and low chlorophyll
  - Distinct changing relationships of chlorophyll with flow by station