



# Simple vs. Complex Modeling: Choosing the Appropriate Level of Complexity When Using Groundwater Modeling in Remediation

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5/30/2019

# SIMPLE VS. COMPLEX



## SIMPLE MODEL

- Limited domain size
- Few boundary conditions
- Larger grid size
- Limited calibration parameters
- Potentially coarser calibration statistics
- Potentially less accurate source data
- More general than “site specific”

## COMPLEX MODEL

- More varied domain – potentially region-wide
- Detailed boundary conditions (frequently derived from complex datasets)
- Extensive calibration
- Potentially tighter calibration statistics
- Potentially more accurate, or detailed data sources
- Typically tailored to “real world” site conditions

# COMPLEXITY PROS AND CONS



## Simple Model Considerations

- Simple to construct
- Quick to calibrate
- Cheaper
- Faster
- More cost-effective
- Lacking in detail
- Could be driven by stakeholders
- Typically less “believed” by stakeholders

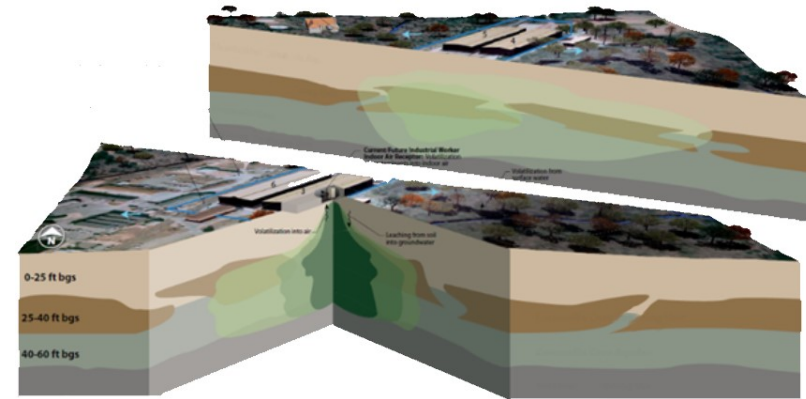
## Complex Model Considerations

- More detailed
- Typically have a “tighter” fit to observed data
- Potentially overemphasizing parameters
- Potential for “overfitting”

- Every piece of additional design increases the complexity of the system
- Each level of complexity increases the chance for model errors due to unforeseen interactions

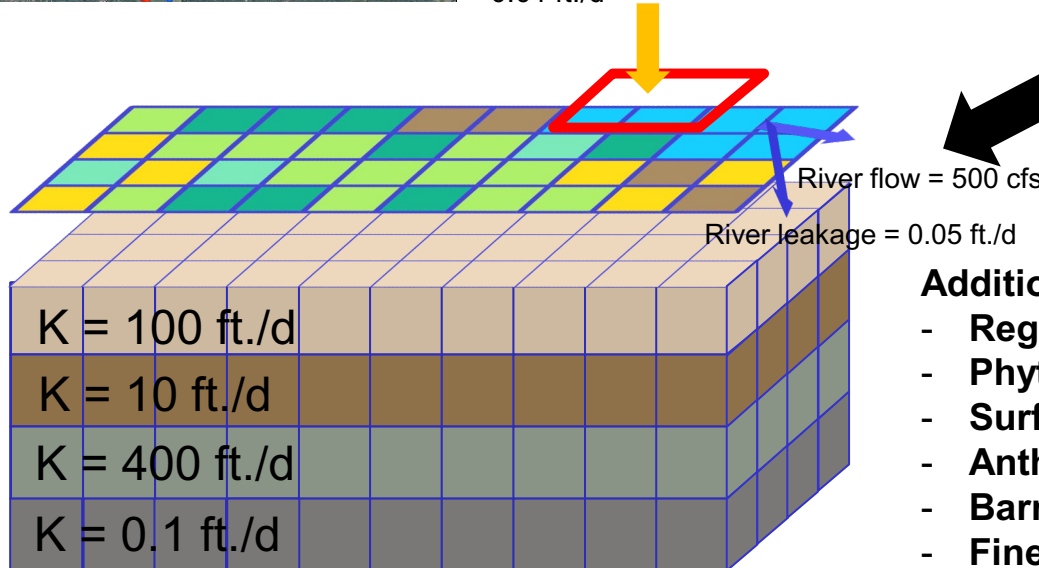
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# HOW MODELS BECOME SIMPLE OR COMPLEX



Source infiltration = 0.01 ft./d

Water level = 10 ft.



## Additional CSM considerations:

- Regional Pumping
- Phytoremediation withdrawals
- Surface lakes
- Anthropogenic infiltration
- Barrier injections
- Fine geologic layering
- Etc.

# ADDED COMPLEXITY AT EVERY STEP



- **Step 1: Construct a CSM**
- **Step 2: Convert the CSM into a groundwater model**
- **Step 3: Calibration**

**Calibration: The adjustment of estimated parameters to “best fit” to known data**

- **Manual calibration**
- **Automated calibration**
- **Combination of both**

**Table 1**

**Guidelines for Effective Model Calibration (Hill and Tiedeman in press; modified from Hill 1998)**

Develop the model

1. Apply the principle of parsimony (start very simple; build complexity slowly)
2. Use a broad range of information (soft data) to constrain the problem

Maintain a well-posed, comprehensive regression problem  
Include many kinds of data as observations (hard data) in the regression

Use prior information carefully

Assign weights that reflect errors

Encourage convergence by improving the model and evaluating the observations

Consider alternative models

Test the model

Evaluate model fit

Evaluate optimized parameter values

Potential new data

Identify new data to improve processes and properties governing system dynamics

Identify new data to improve predictions

Prediction accuracy and uncertainty

Evaluate prediction uncertainty and accuracy using deterministic methods

Quantify prediction uncertainty using statistical methods

# COMPLEXITIES IN CALIBRATION

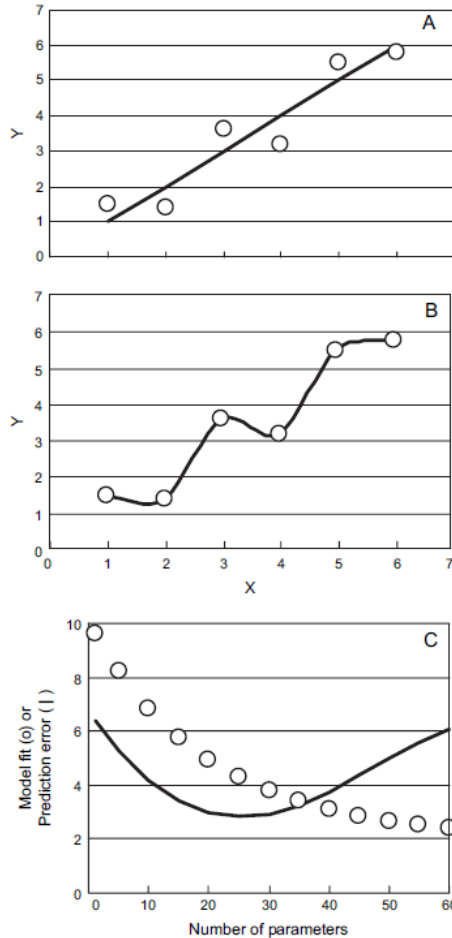


Figure 2. (A) Data with a true linear model; “model fit” is the fit of the model to observations. (B) The same data with an overly complex model with diminished predictive capability. (C) Schematic diagram showing a tradeoff between model fit to observations and prediction accuracy with an increasing number of parameters.

- **Concerns to consider:**
  - Interference between K and recharge
  - Over-specifying boundary conditions
  - Over-tightening parameters to “known values”
  - Too-simplistic hydrogeologic interpretation
  - Too-Complex hydrogeologic interpretation
  - Too far from “known” water levels
  - Too close to “known” water levels
- **Only go as complex as the data allows**
  - How sensitive are the parameters?
  - Overfitting = bad modeling
  - Is the parameter vital in understanding the system?
  - Does the complexity assist in answering the question posed?

# DATA LIMITATIONS



Example:

Well measurements were collected with a sounder with an accuracy of +/- 0.2 feet.

Impact: A “perfect fit” for an observed measurement of 10 feet could be between 9.8 and 10.2 feet within the simulation. Therefore any prediction within the model must be within the “bounds” of this error.

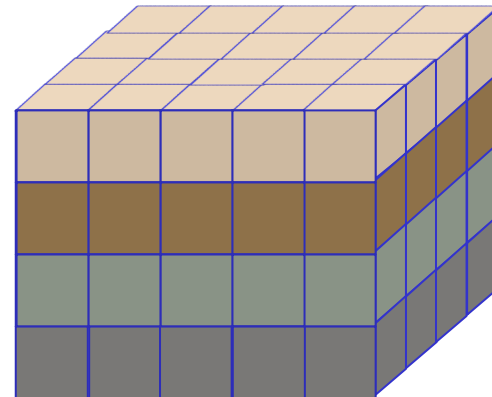
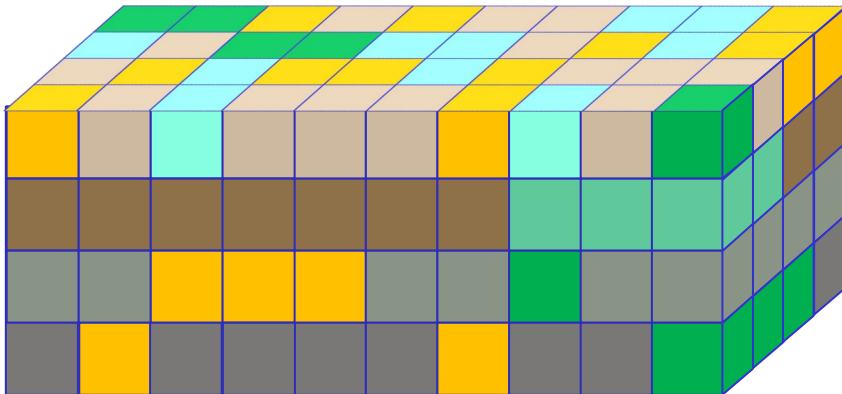
# SIMPLE VS. COMPLEX

## A TALE OF TWO MODELS

$$A + B = C$$

$$\frac{P_1}{\rho} + \frac{v_1^2}{2} + gz_1 = \frac{P_2}{\rho} + \frac{v_2^2}{2} + gz_2$$

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} = 0$$



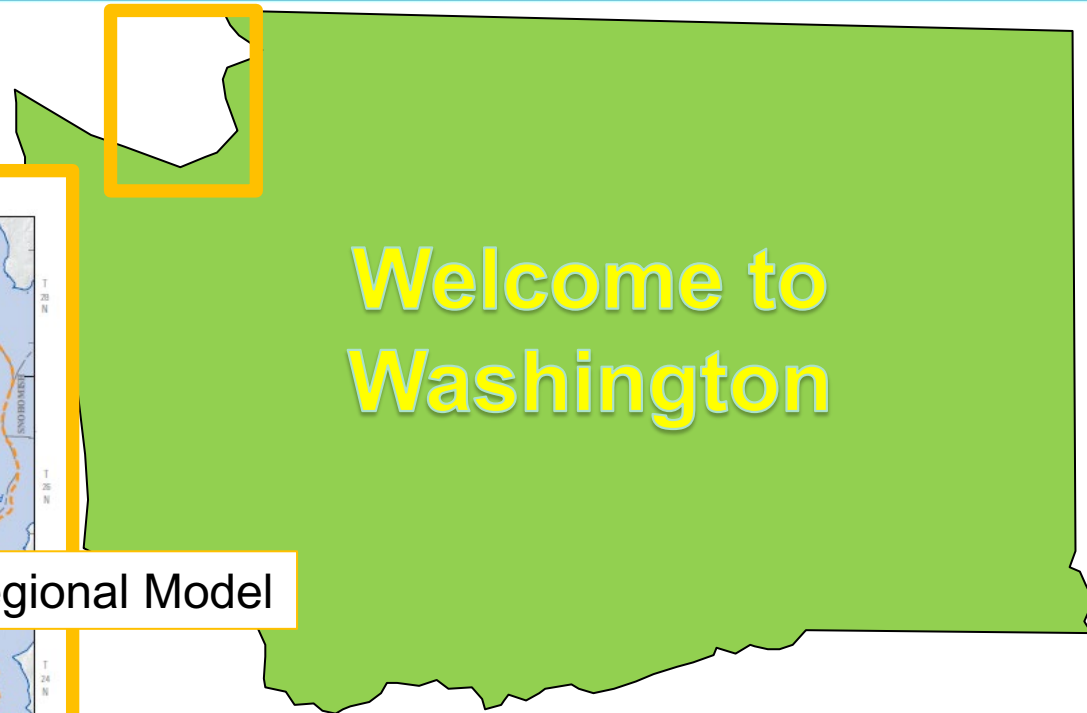


# WASHINGTON FACILITIES



Two Installations, located within the Kitsap Peninsula Group

- Bo
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Welcome to Washington

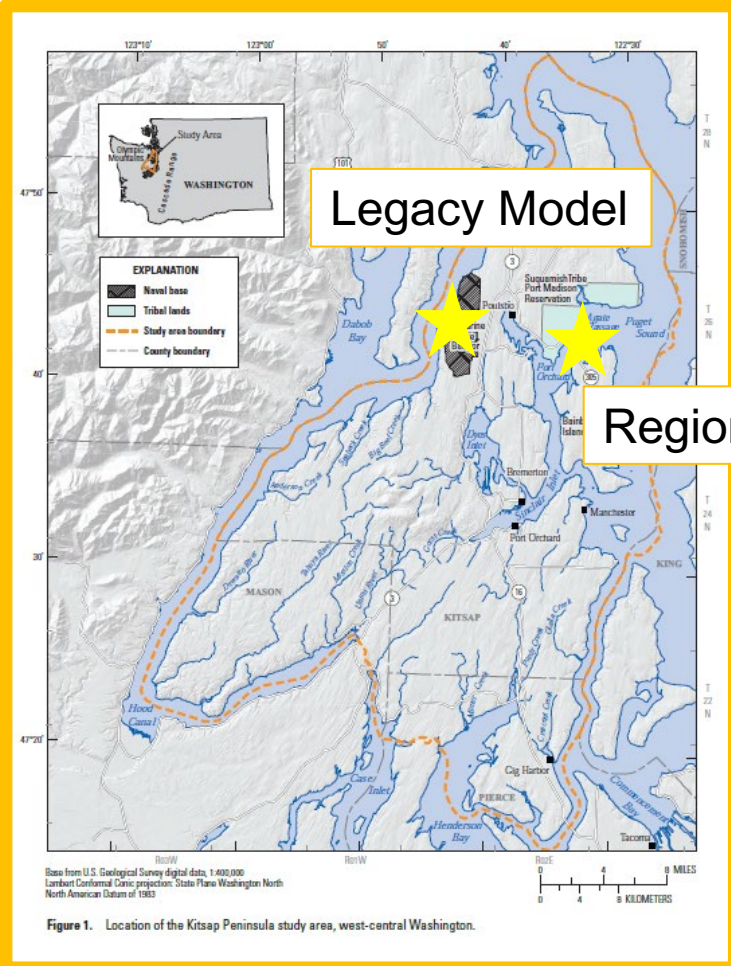


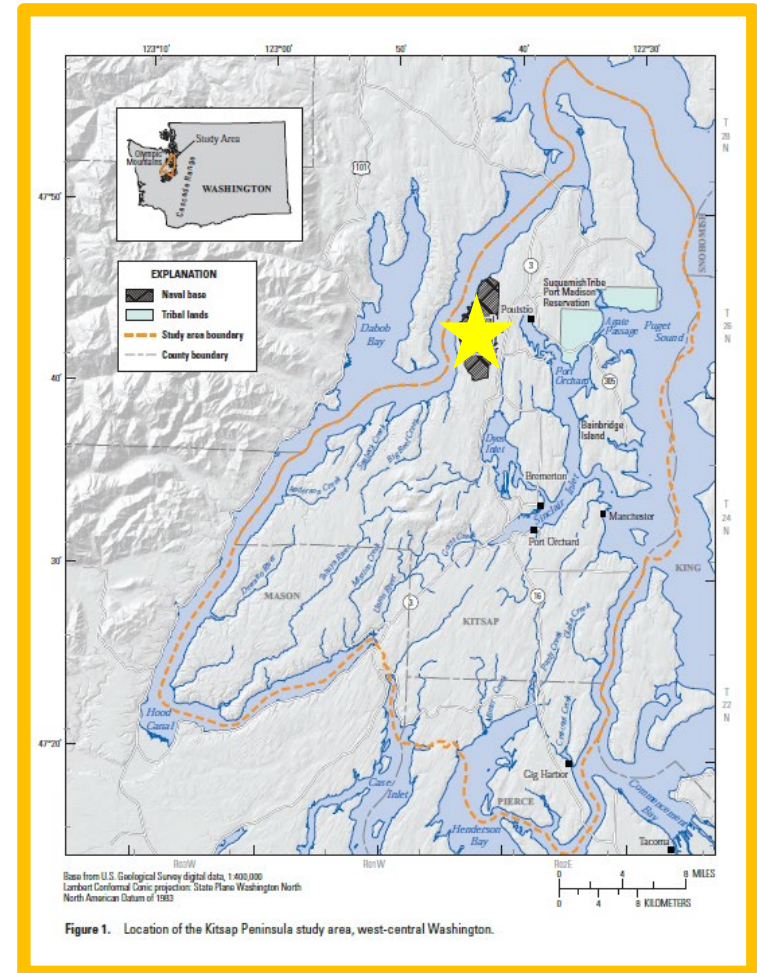
Figure 1. Location of the Kitsap Peninsula study area, west-central Washington.

Via: Welch, 2016 (USGS)

# NAVAL BASE KITSAP



**When A Simpler Model Would  
be Best  
(even if the site is complex)**



Via: Welch, 2016 (USGS)

# LOCATION OU 2, SITE F



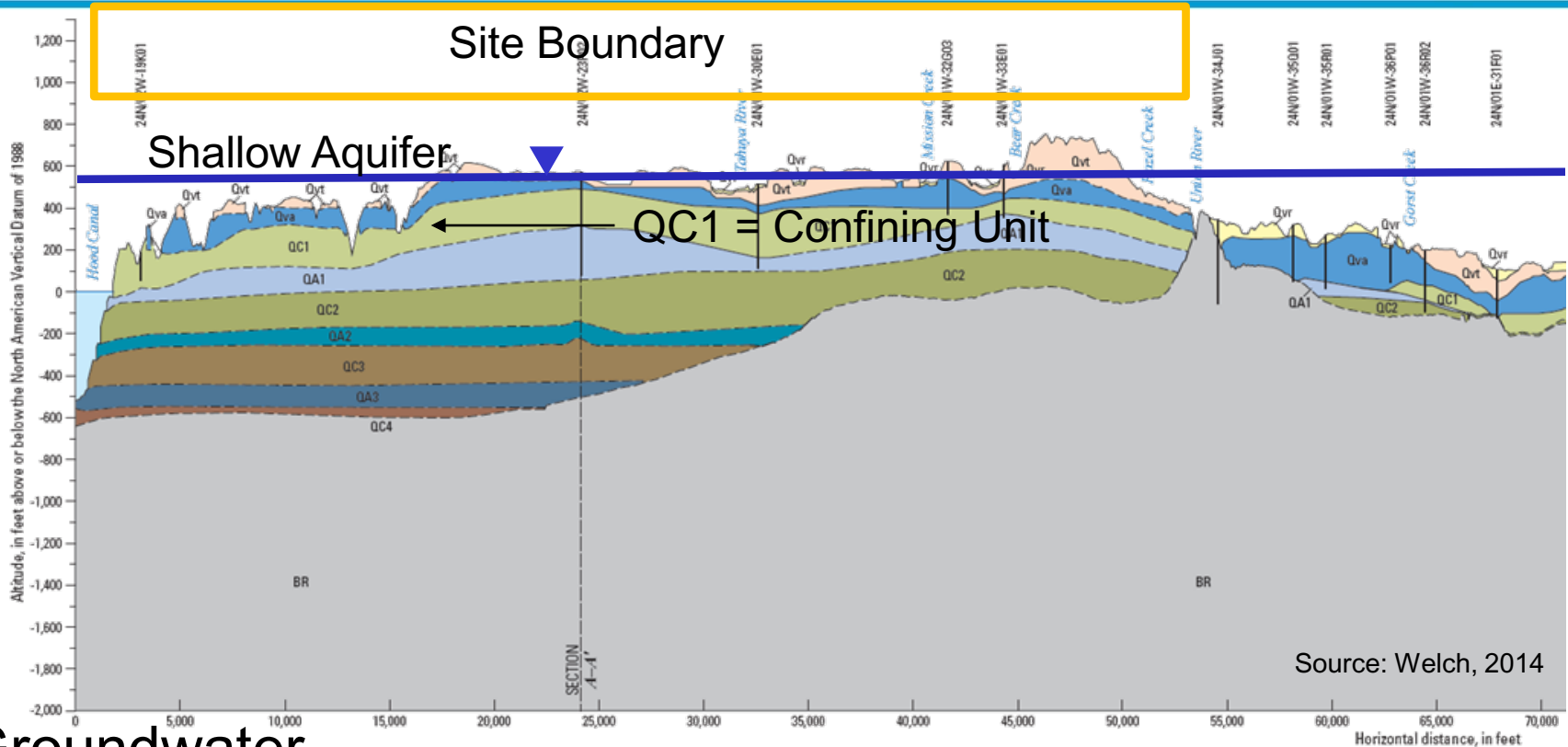
~0.75-acre site

Surrounded by large forested area

Closed basin with no natural drainages

Hood Canal – 1.5 miles W of site

# LOCATION OU 2, SITE F



## Groundwater

Shallow Aquifer: ~50 feet BGS, 60-100 feet thick. Unconfined, within stratified sand/silt deposits.

Sea Level Aquifer: Confined by aquitard 80-100 feet below shallow aquifer. Not impacted. Water supply for Vinland.



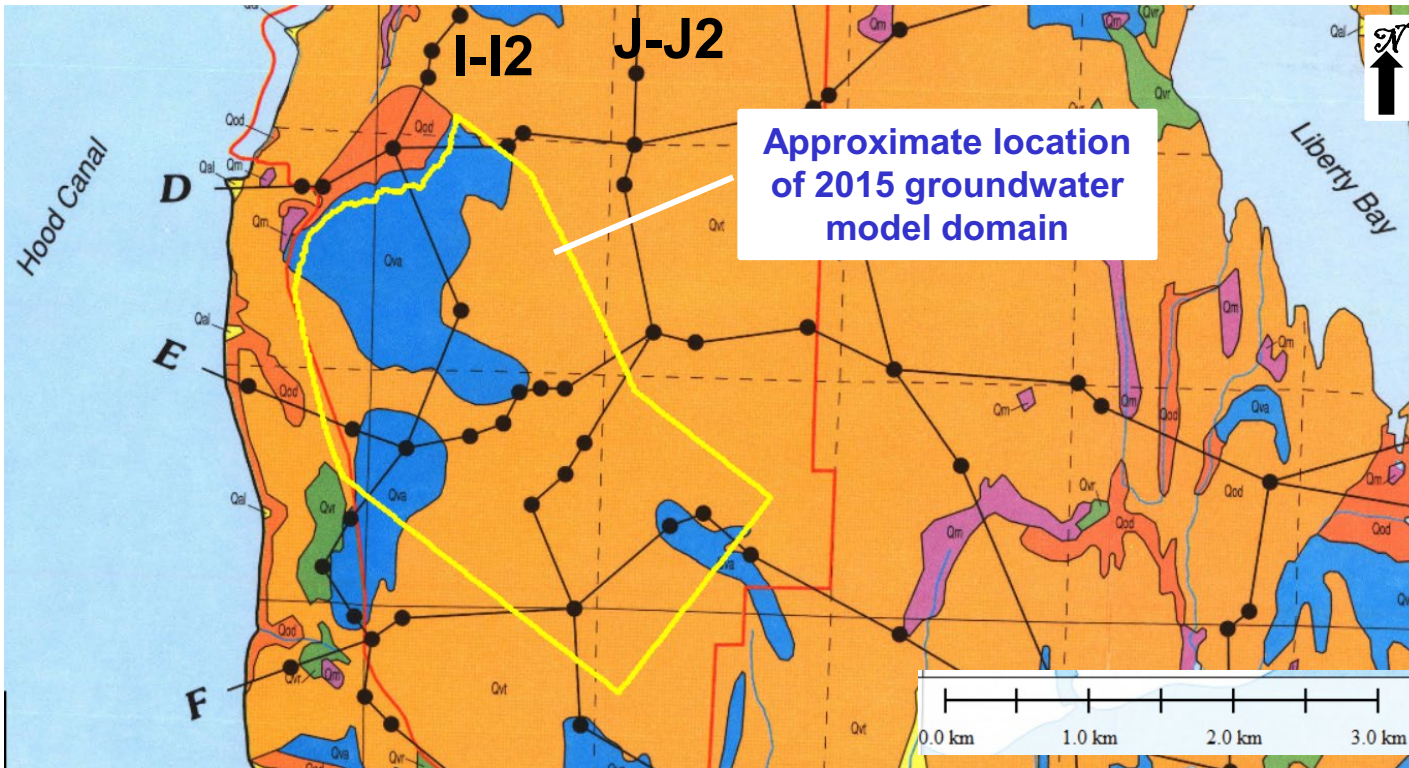
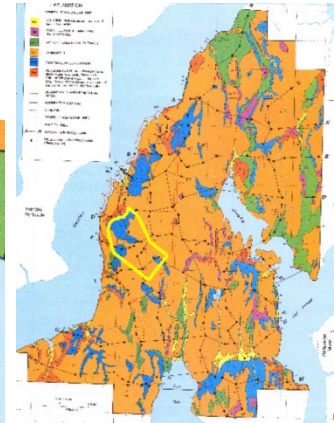
# OU 2 – SITE F HISTORY



## Former Wastewater Location

- 1960-~1972: Unlined lagoon and overflow ditch used for ordnance demilitarization wastewater disposal
  - **Created a subsurface contamination problem**
- 1972: 500 ft<sup>3</sup> soil excavated from lagoon; burned at a different location **but the problem was not solved**
- 1980: Lagoon area backfilled and covered with asphalt
- 1987: OU2 added to EPA NPL
- 1991: Interim Remedial Action ROD signed
- 1994: Final ROD signed
- 1999: Initial Groundwater model constructed
- 2015: Groundwater Model used to address plume movement

# LEGACY MODEL DOMAIN



## EXPLANATION

### GENERALIZED GEOLOGIC UNIT

- Qal** ALLUVIUM - includes stream, beach, and landslide deposits
- Qm** MARSH DEPOSITS - includes bog deposits and peat
- Qvr** VASHON RECESSONAL OUTWASH
- Qvt** VASHON TILL
- Qva** VASHON ADVANCE OUTWASH
- Qod** OLDER DEPOSITS - includes early Vashon glaciolacustrine deposits, Possession Drift, and Whidbey interglacial deposits (Qvgl, Qvp, and Qng, respectively, on plate 2), and pre-Fraser deposits, undifferentiated

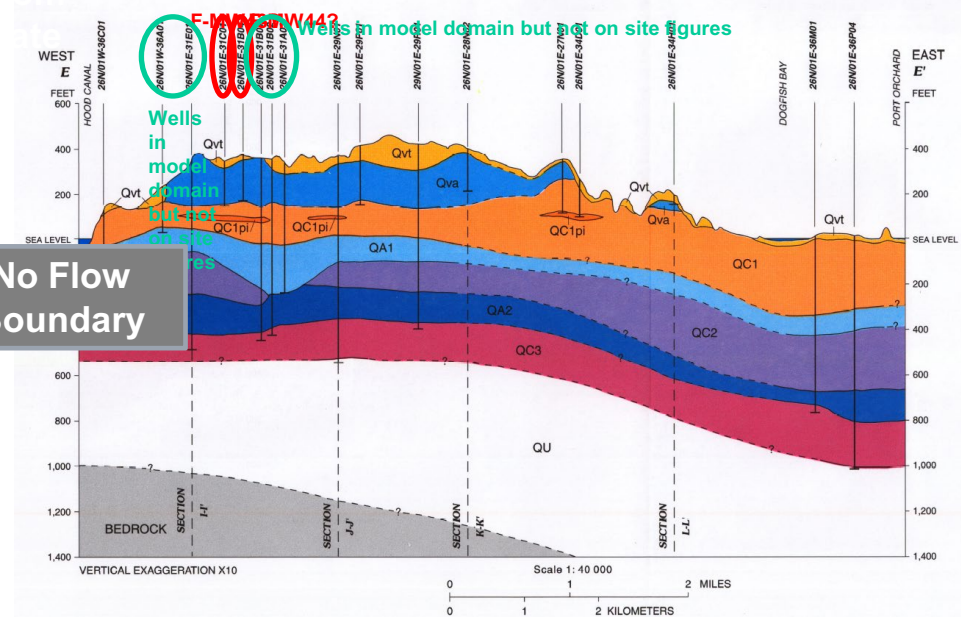
Modified from: Kahle 1998

# LEGACY MODEL



Statistic	Legacy Model
Residual Mean	0.02
Absolute Residual Mean	0.72
Residual Std. Deviation	1
Sum of Squares	3,600
RMSE	1
Min Residual (ft.)	-4.55
Max. Residual (ft.)	5.89
Number of Observations	3,671
Range (ft.)	24.07
Scaled Residual Mean	0.10%
Scaled Absolute Residual Mean	3.00%
Scaled Residual Std. Dev	4.10%
Scaled RMSE	4.10%

From

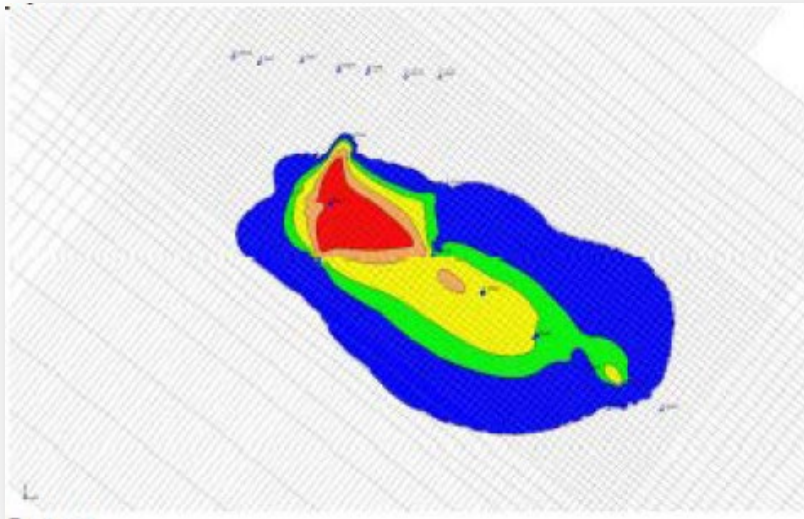


General Head Boundary

Same K through model layers except at the bottom where it was lower

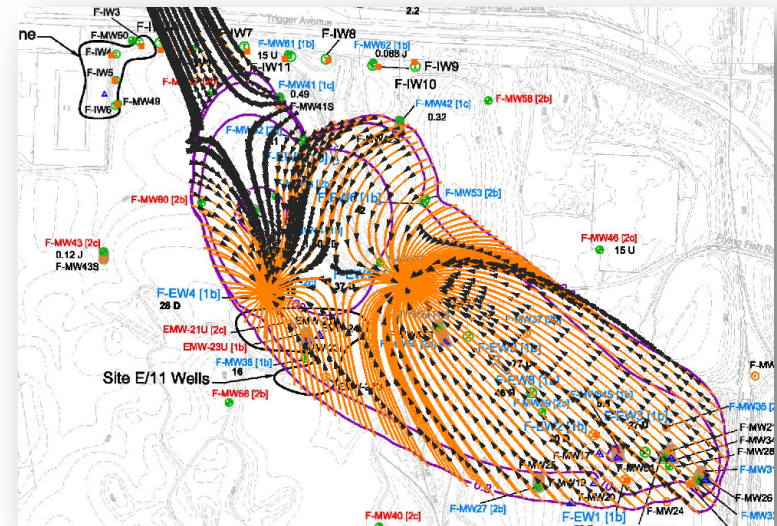
# LEGACY MODEL - CONCERNS

- Model fit well, but did not mimic known “bend” in observed contaminants
- After review, the general head boundaries were determined to be forcing the water in the system to flow directly across the site, rather than curving
- Therefore modelers simplified the model by removing the general head boundaries and placing drains at the northern edge



2015 model from USACE 2015

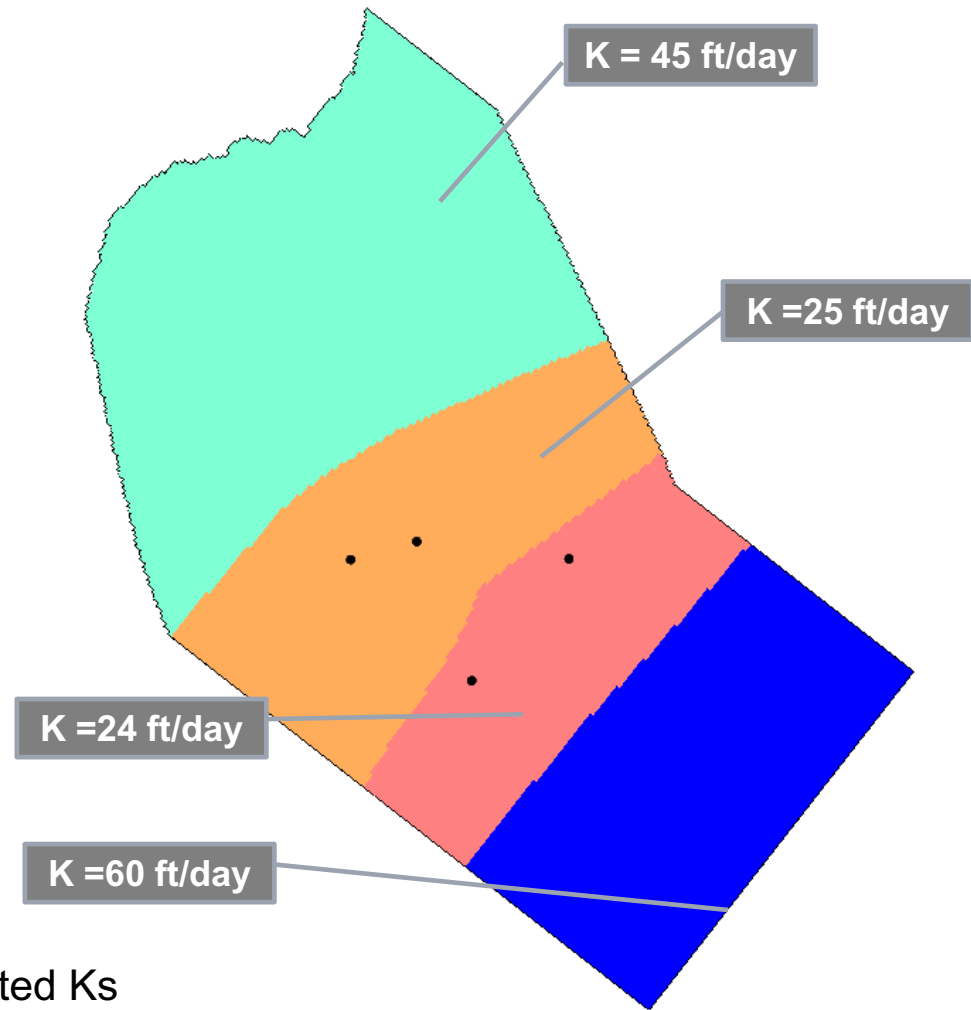
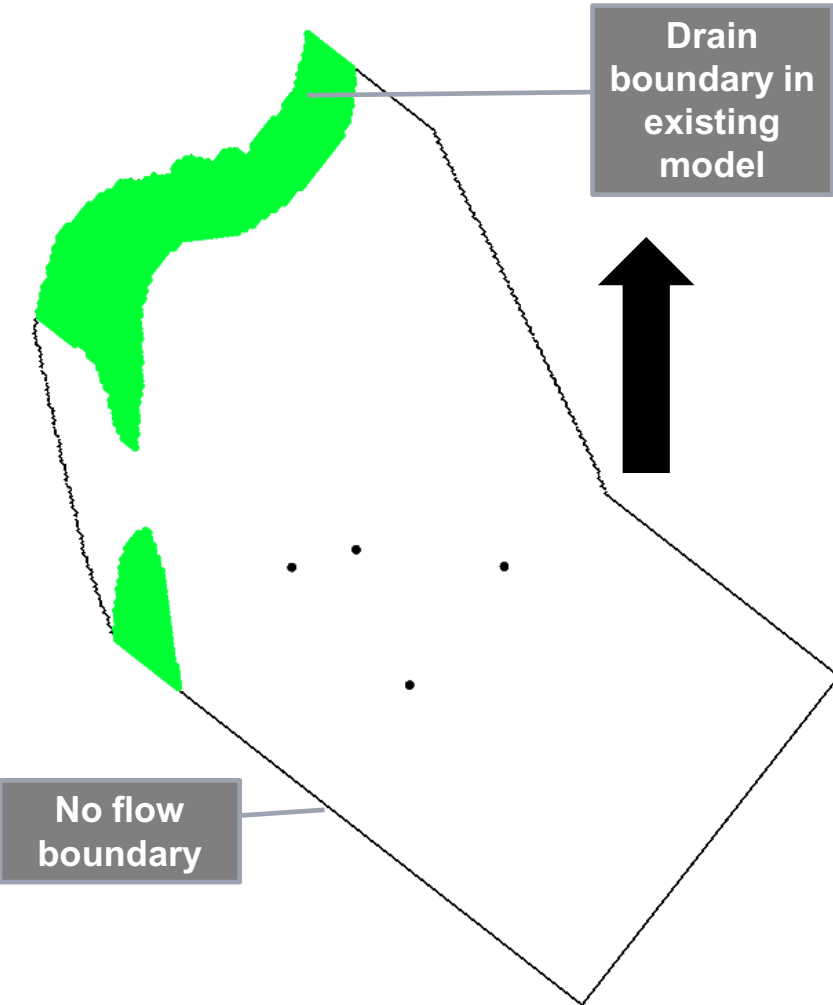
VS



Updated model from SEALASKA (Via GSI) 2018



# SIMPLIFIED MODEL UPDATES

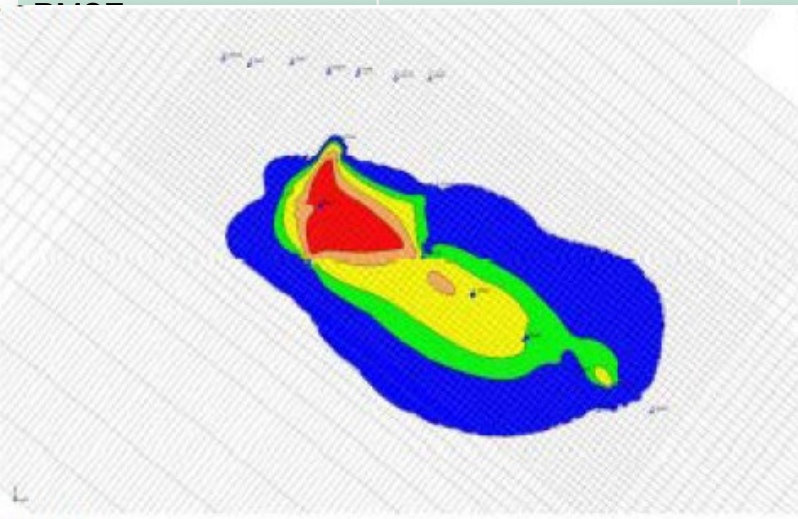


Modified Boundary conditions, recalibrated Ks

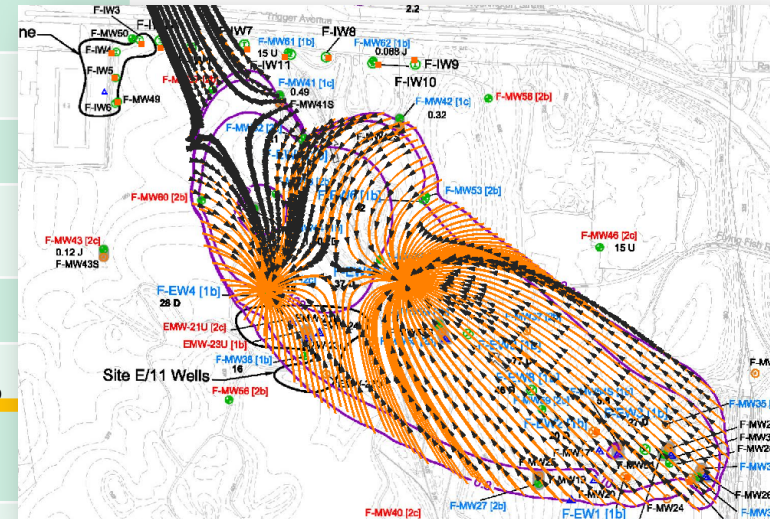
# MODEL COMPARISONS

Statistic	Legacy Model	Simplified Model
Residual Mean	0.02	-0.6
Absolute Residual Mean	0.72	1.87
Residual Std. Deviation	1	2.42
Sum of Squares	3,600	38,090

**RESULT:**  
more realistic transport with simpler boundary conditions



2.49  
-12.75  
16.31  
6,132  
24.07  
-2.50%  
7.80%



Scaled Residual Std. Dev.	4.10%	10.40%
Scaled RMSE	4.10%	10.40%

2015 model from USA CE 2015

Updated model from SEALASKA (Via GSI) 2018

# SITE CONCLUSIONS

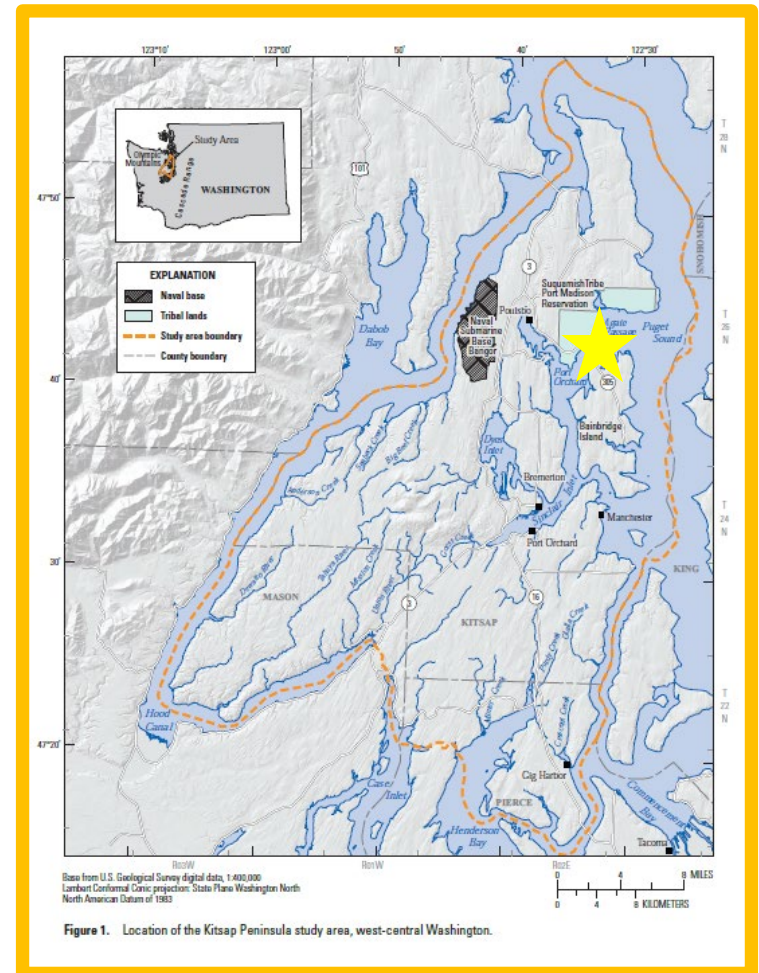


- **Original model fit typical modeling statistics**
  - **Model may have been “over fit” for transport purposes**
- **Simplifying the model boundary conditions allowed for more flexibility in flow directions**
  - **This allowed for a better transport model**

# NAVAL AIR STATION KEYPORT



## When More Complexity is Better



Via: Welch, 2016 (USGS)

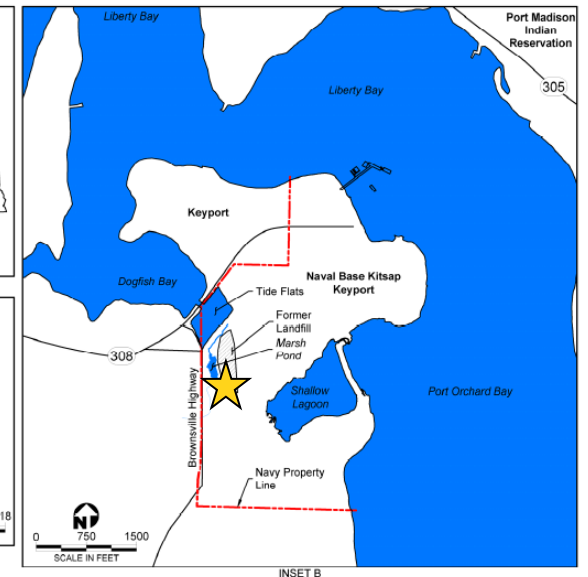
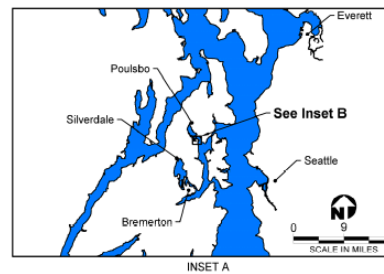
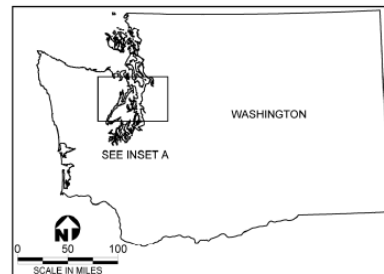
# LOCATION OU 1



~9 acre former landfill site

Surrounded by large forested area and outflowing to surface water to the south and the east

Flows to the Dogfish Bay through tidal flats





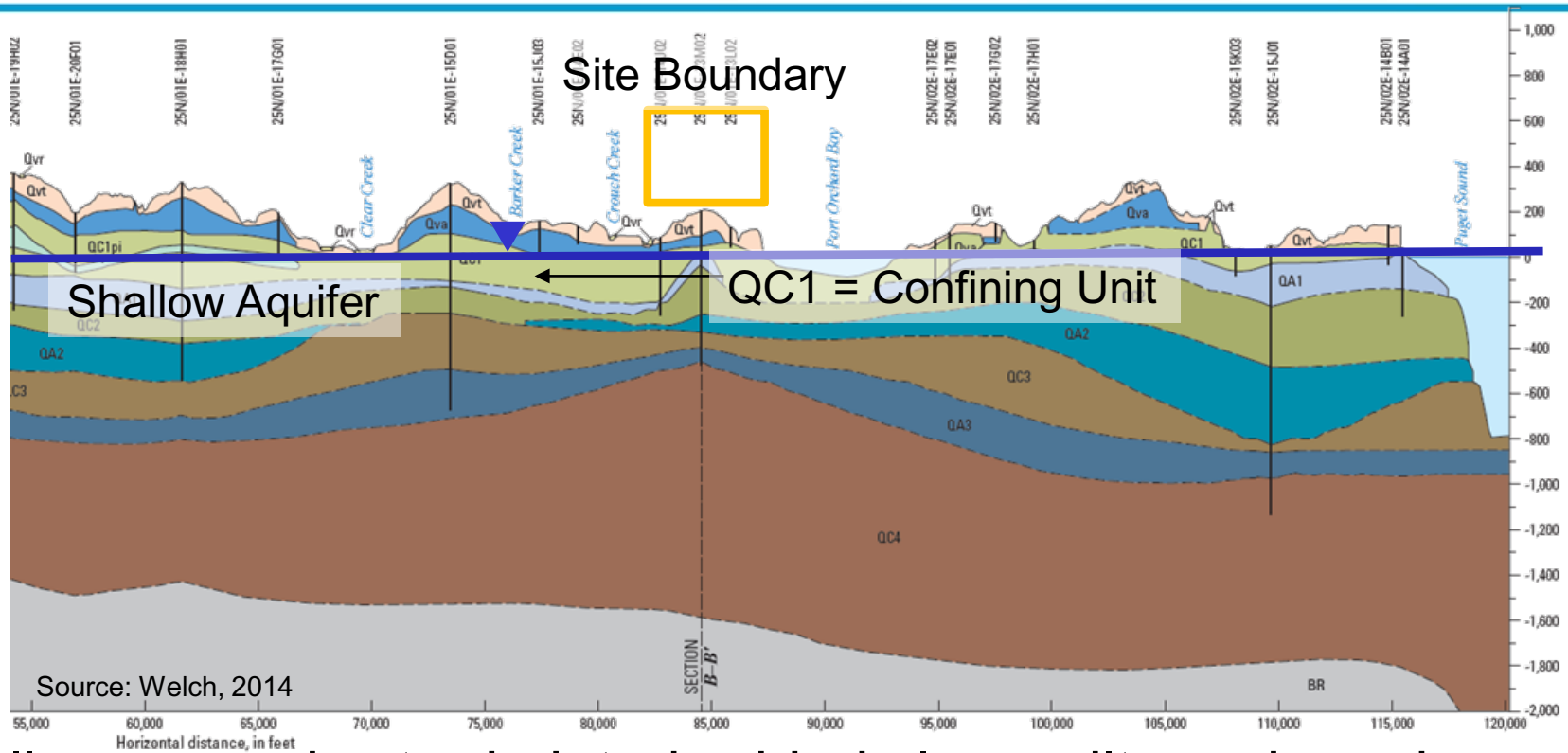
# OU 1 – SOUTH PLANTATION HISTORY



## Former Unlined Landfill and Disposal Location

- 9-acre former landfill in western part of installation (Keyport Landfill)
- Received domestic and industrial wastes from 1930s to 1973 when landfill was closed
- Burn pile and incinerator operated in the northern end of landfill from 1930s to 1960s
- Received paint wastes and residues, solvents, residues from torpedo fuel (Otto fuel), WWTP sludge, pesticide rinsate, plating waste, etc.
- Landfill occupies former marsh land that extended from tidal flats to shallow lagoon
- Landfill cover consists of soil, asphalt, and concrete

# LOCATION OU 1 – REGIONAL GEOLOGY



Shallow groundwater in interbedded clays, silts and sands

Hydrogeologic units

- Unsaturated zone
- Upper aquifer (sandy material with silt units)
- Middle aquitard (absent in the central, eastern, and northern parts of landfill)
- Intermediate aquifer (sand with some gravel and significant silt)

# REGIONAL MODEL DOMAIN

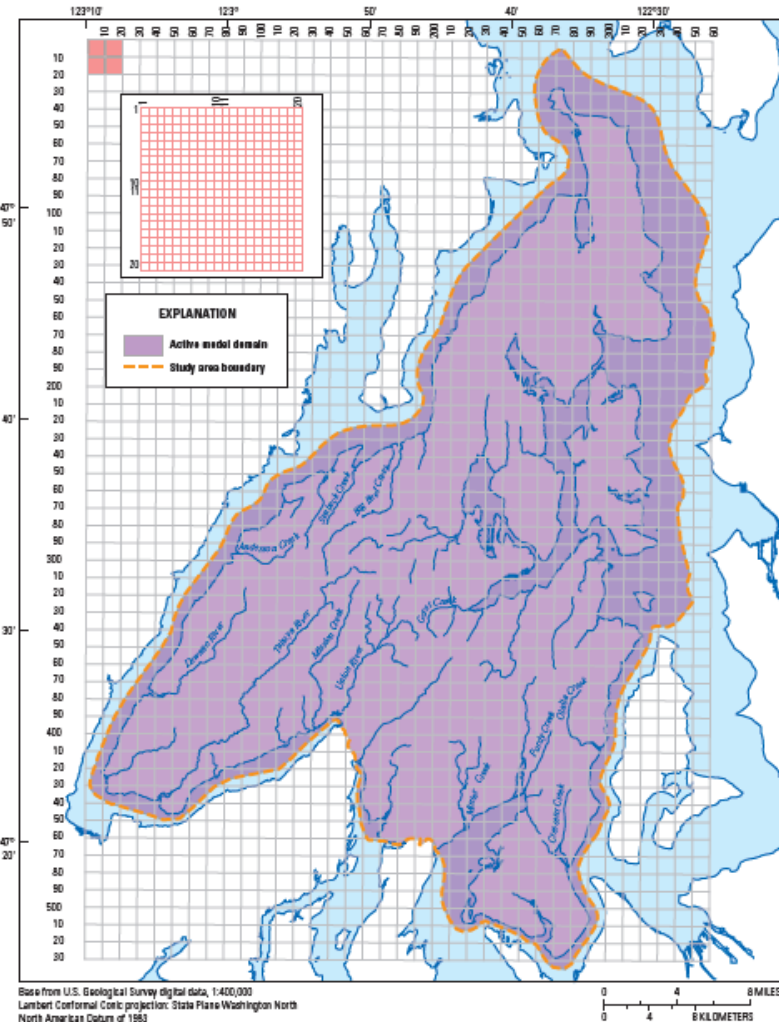


Figure 2. Location and extent of the groundwater model grid, west-central Washington. The insert depicts the detailed horizontal discretization of the 20 rows and 20 columns of the grid  
via. Welch, 2016 (USGS)

- Constructed in 2016 by USGS
- 14 layers of variable thickness
  - One layer for each aquifer unit
- 500 x 500 ft. cells
- General model encompassing over 575 sq. mi.

Statistic	Legacy Model
Residual Mean	3.70
Residual Std. Deviation	47.01
RMSE	47.16
Number of Observations	18,834
Range (ft.)	647.40
Scaled Residual Mean	0.57%
Scaled Residual Std. Dev	7.26%
Scaled RMSE	7.28%

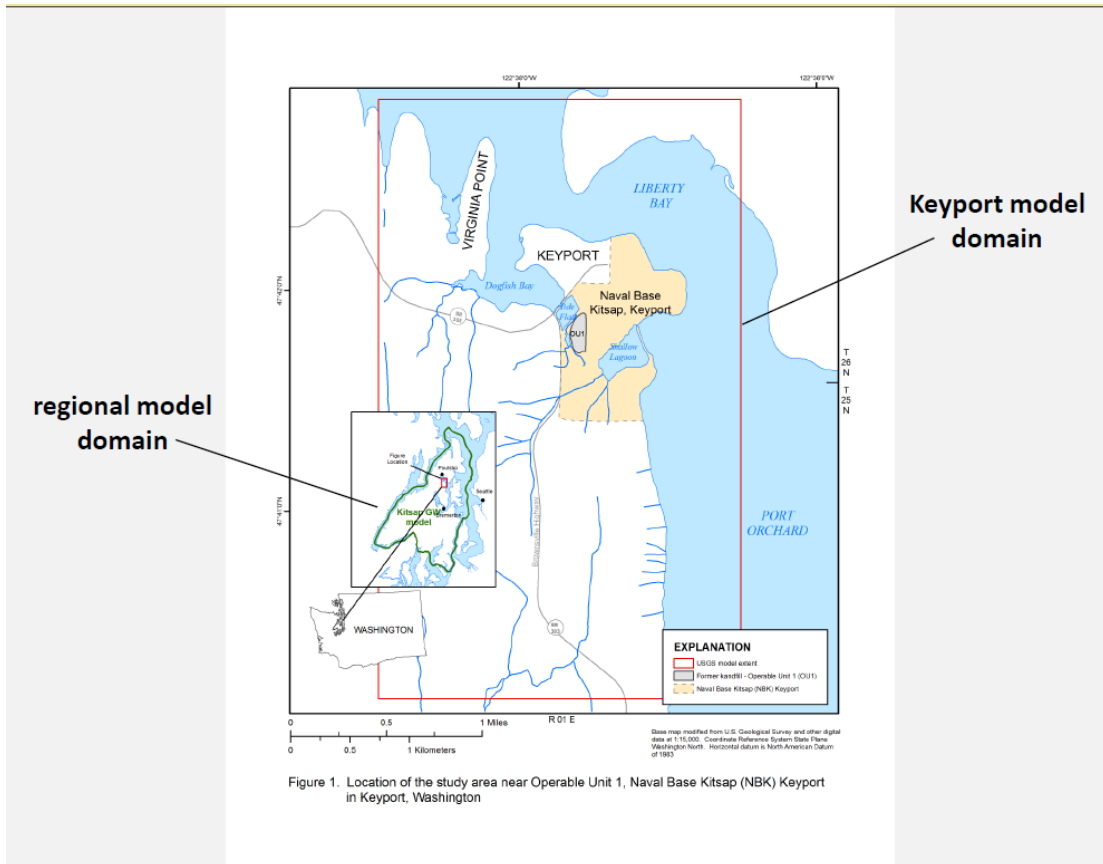


# REGIONAL MODEL - CONCERNS



- **Model fit well regionally, but did not mimic known groundwater divide at the site**
- **Model cell size was too large for transport modeling**
- **Shallow zone not adequately modeled to address the complexities of clays and sands in the subsurface, as well as flows to the local streams**
- **Therefore, a more complex and focused site model was determined to be necessary**

# REFINEMENT OBJECTIVES



- Refine model
  - Cells in site area at 25 ft. x 25 ft.
  - Cells outside AOI at 500 ft. x 500 ft.
- Additional vertical refinement and geologic interpolations in the shallow zone (layer 1)
- Recalibrate with site specific data
- Convert to SEAWAT model
- Calibrate
- Model Transport through groundwater to potential surface water receptors

Via: Yager 2019 (USGS, in-development)

# VERTICAL REFINEMENT



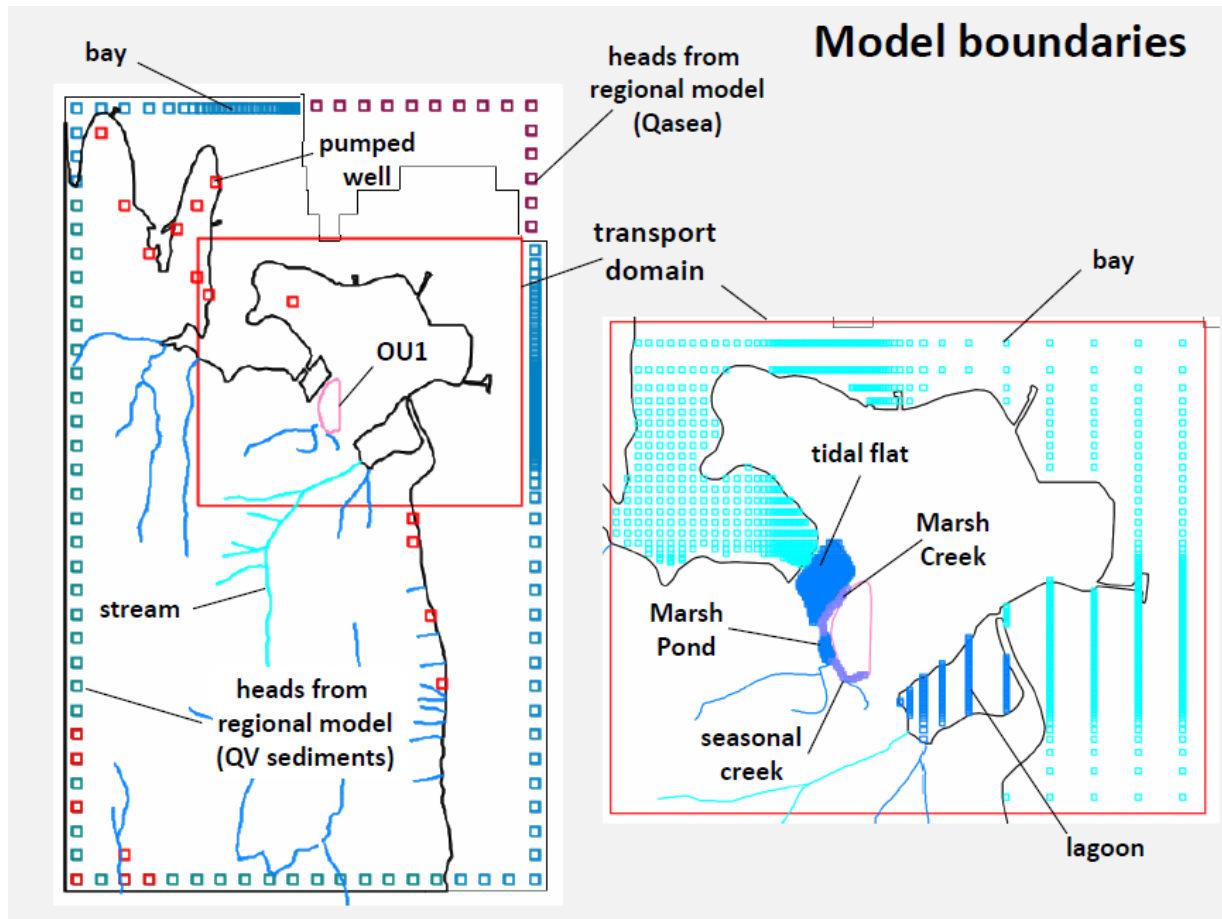
## Model layers

### Keyport model

transport model	flow model	geologic model	USGS Kitsap model (Welch and others, 2014)
Layer 1 - water	Layer 1 - water		
Layer 2	Layer 2	Layer 1 - A, QVr	QVr, Vashon recessional aquifer
↑	↑	Layer 2 - QVm marsh/marine	
QV sediments	QV sediments	Layer 3 - QVt till	QVt, Vashon till confining unit
↓	↓	Layer 4 - QVa upper Aquifer	Qva, Vashon advance aquifer
Layer 11	Layer 11	Layer 5 - QVmc ; middle Semi-confining unit	
		Layer 6 - QVia ; intermediate Aquifer	
	Layer 12 - QC1up	Layer 7 - QC1up	QC1, Upper confining unit
	Layer 13 - QC1pi	Layer 8 - QC1pi	QC1pi, permeable interbeds
	Layer 14 - QC1low	Layer 9 - QC1low	QC1, Upper confining unit
	Layer 15 - QA1	Layer 10 - QA1	QA1, Sea-level aquifer

Via: Yager 2019 (USGS, in-development)

# REFINED MODEL DOMAIN



Via: Yeager 2019 (USGS, in-development)

# CALIBRATION - CONCERNS

Via: Yager 2019 (USGS, in-development)

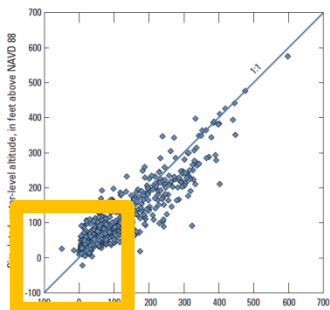
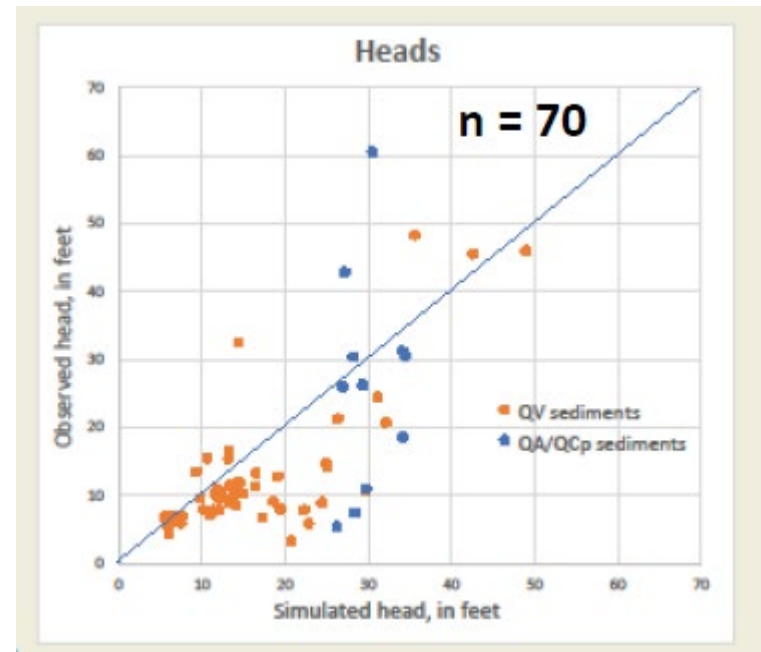
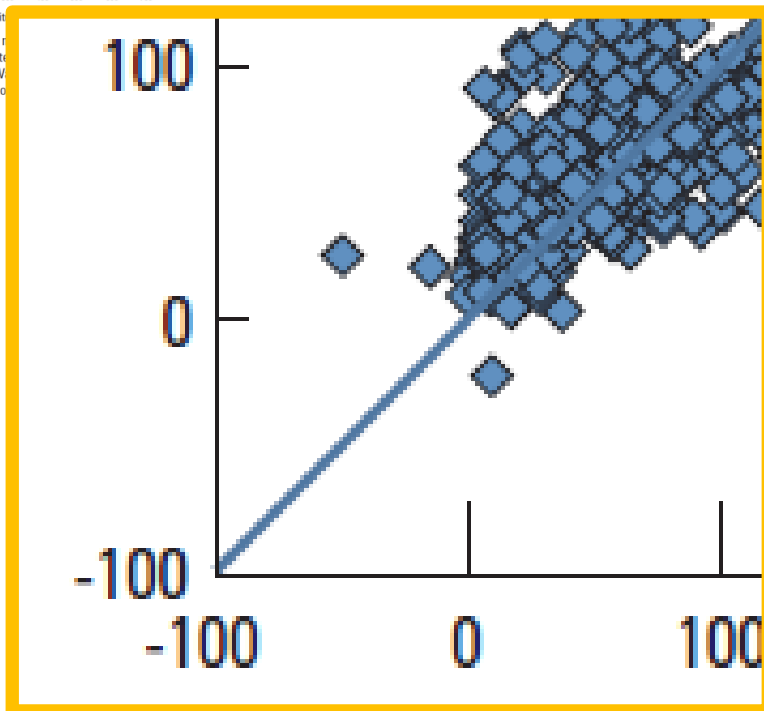


Figure 5. Simulated and measured altitudes in the groundwater on the West-Central Florida Peninsula, west-central West Florida, American Vertical Datum of 1988.



**(Still in Final Calibration)**  
**Model Calibration: RMSE at 15%**  
**Average error: 9 ft. (vs. 47 ft.)**  
**Range in heads 60 ft. (vs. 647 ft.)**

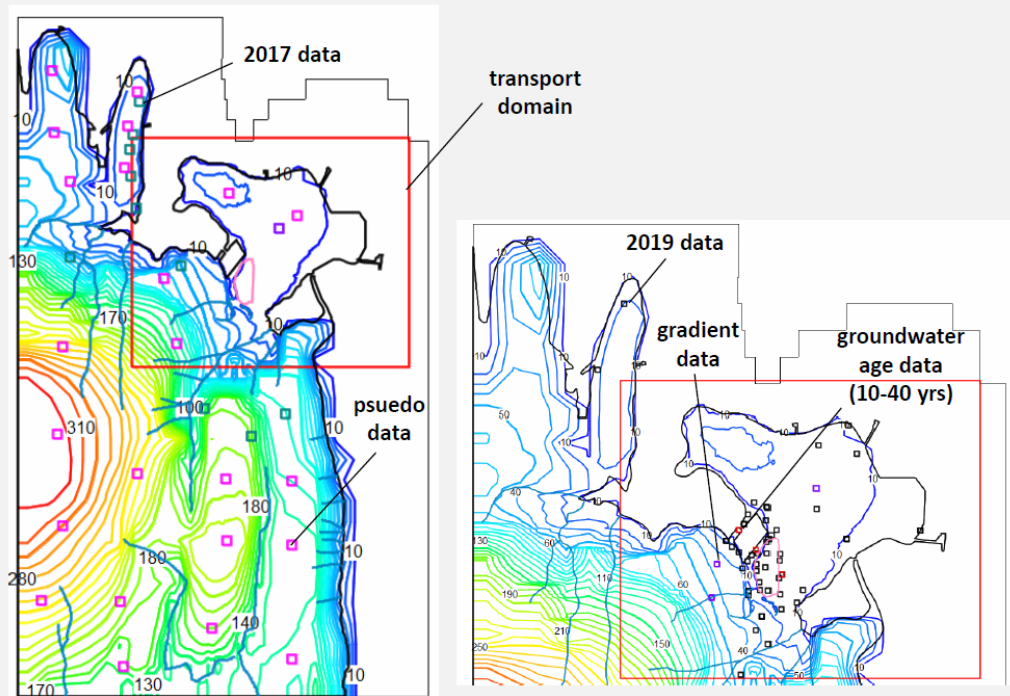
Via: Welch, 2016 (USGS)

# MODEL COMPARISON – WATER LEVELS

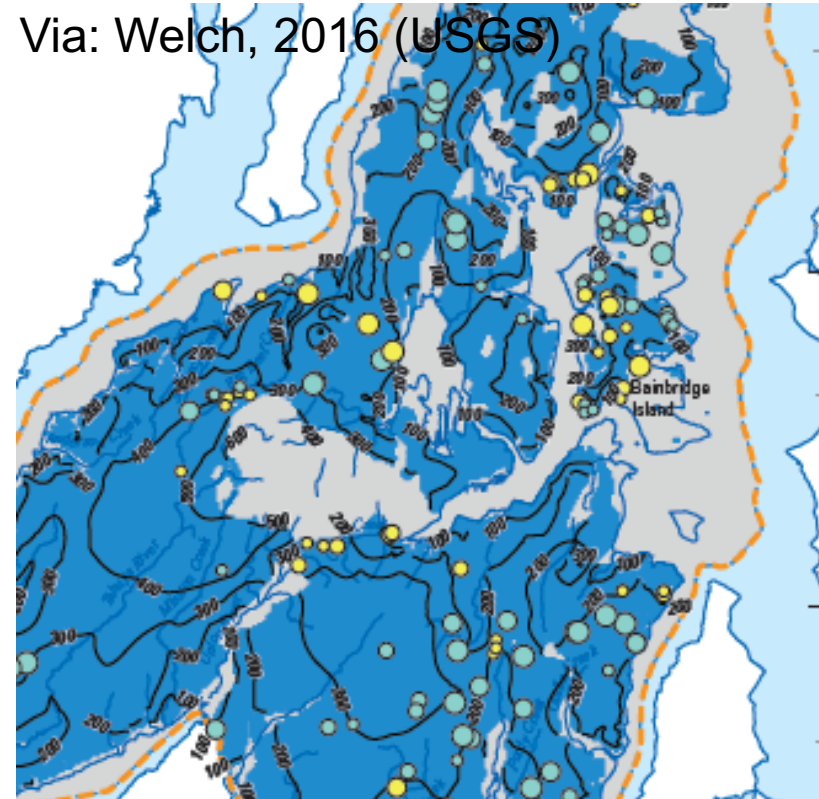


Via: Yager 2019 (USGS, in-development)

Simulated water table



Via: Welch, 2016 (USGS)



**Water levels too coarse in regional model, however refined model provides better clarity for subsequent transport modeling**

# SITE CONCLUSIONS



- **Refined model still in construction, however it was able to address flow directions at the site with more detail than the regional model**
- **Allows for differential densities (important in a tidal zone)**
- **Implemented more refined geology and boundary conditions**
- **Allowed transport questions to be addressed at this site (a vital tool for the RPM)**

# WASHINGTON SUMMARY



- **Both locations optimized existing groundwater models to address new questions**
  - one simplified to address flow direction considerations
  - one refined and added complexity to address local shallow zone dynamics
- **While model adjustments provided less specific “fits” than were provided with the original models, the dynamics under consideration improved**
  - simplifying increased the impacts of pumping on particles to transport COCs throughout the domain, mimicking “real world” observations
  - increasing complexity and cell refinement allowed for a better localized fit, with field-observed groundwater divides
- **Both models provided “better” results than the original models for the modified questions posed**



# POTENTIAL QUESTIONS



Question	Simpler	More Complex
What is the extent of the area of interest?	Small domain; simplified regional flows	Complex geology/hydrology; large regional considerations
What grid size do you need?	Large cells are fine	Refined/small cells needed
Are you considering additional modeling (i.e. transport)?	Maybe, but not complex modeling	Yes
What is your budget?	Relatively small	Medium to large
What is the deadline?	Really soon, we need an answer now	We have months to years to determine the best result
What data do you have?	We have water levels, some geology, and generalized flow conditions and/or stream measurements	We have detailed flow direction measurements, 3D geologic interpretations, continuous sampling of water levels, and surface discharge

**Depending on what the specificity of your questions, the availability of reliable and accurate data, and the timeline/budget should drive the complexity of your system**

# FINAL CONSIDERATIONS



## Garbage in = Garbage out

- **Complexity can both add to —and detract from— the accuracy of your model**
- **Determining the level of complexity you need is key to adequately modeling your system**
  - **The level of complexity needed may change through time, requiring an optimization or modification in your interpretation of your system**
- **Sometimes a simple model may be the best option, even if the result is more conceptual than site-specific**



# Thank you

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