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

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SIMPLE VS. COMPLEX

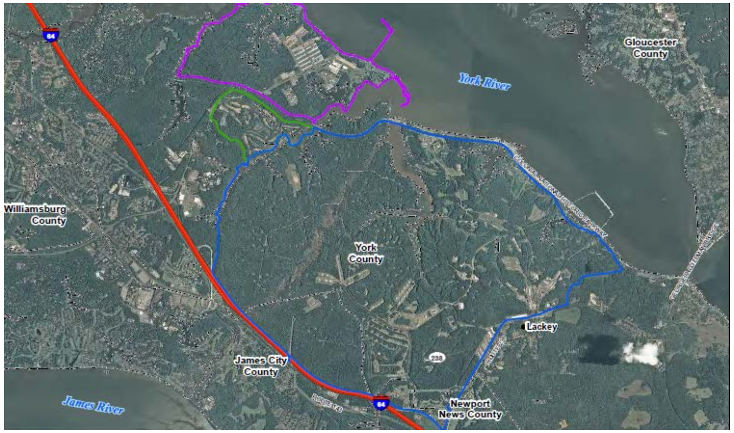
SIMPLE MODEL	COMPLEX MODEL
•Limited domain size •Few boundary conditions •Larger grid size •Limited calibration parameters •Potentially coarser calibration statistics •Potentially less accurate source data •More general than “site specific”	•More varied domain – potentially region-wide •Detailed boundary 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

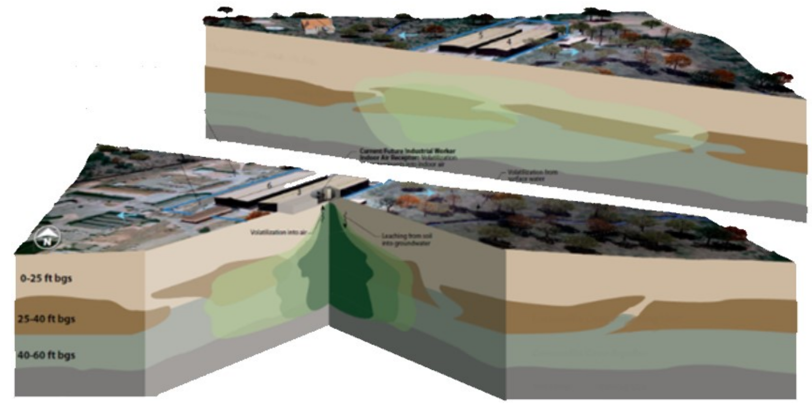
COMPLEXITY PROS AND CONS

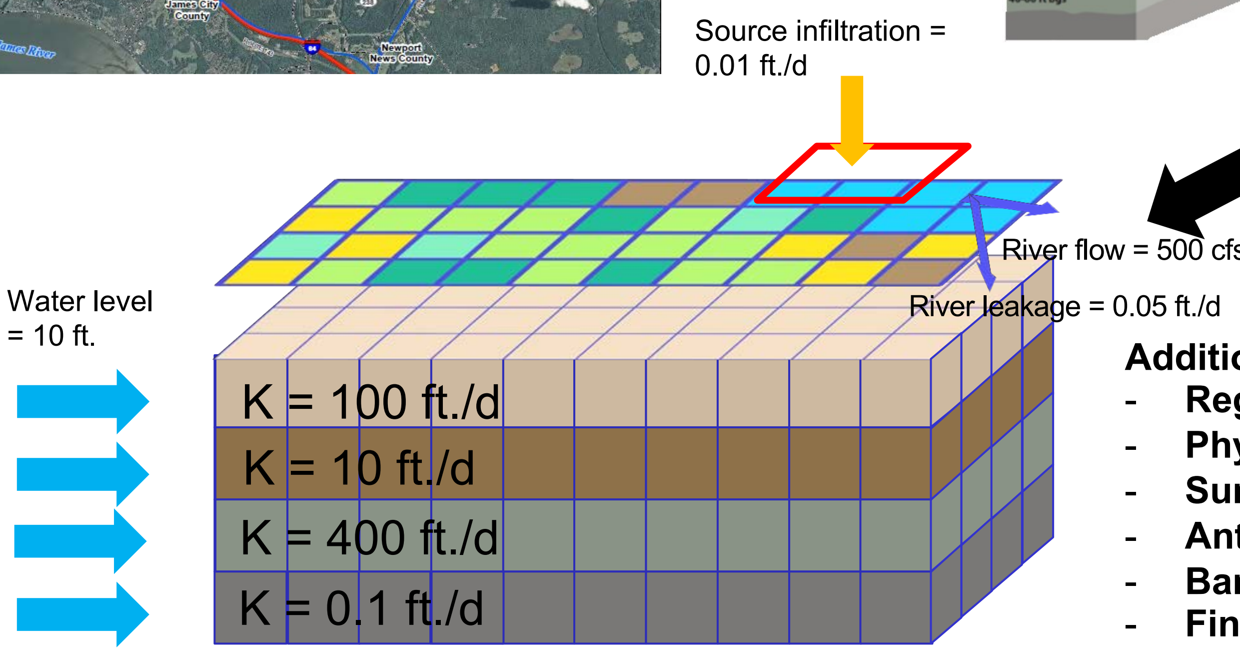
Simple Model Considerations	Complex Model Considerations
•Simple to construct •Quick to calibrate •Cheaper •Faster re •More co •Lacking •Could be drivers •Typically less "believed" by stakeholders	•More detailed •Typically have a "tighter" fit to observed data ng •Potentially overemphasizing parameters •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

HOW MODELS BECOME SIMPLE OR COMPLEX







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

Hill, 2006

COMPLEXITIES IN CALIBRATION

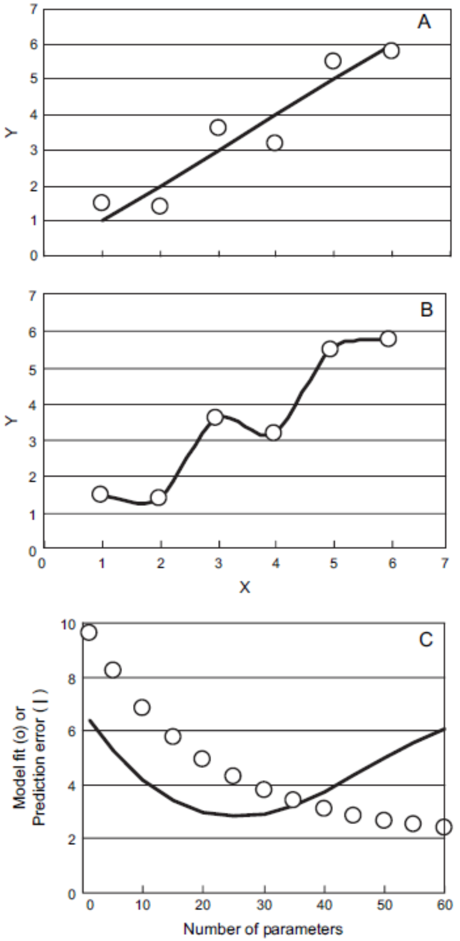


Figure 2. (A) Data with a true linear model; "model fit" is the fit of the model to observations. (B) The same data with an overly complex model with diminished predictive capability. (C) Schematic diagram showing a tradeoff between model fit to observations and prediction accuracy with an increasing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

Hill, 2006

DATA LIMITATIONS

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

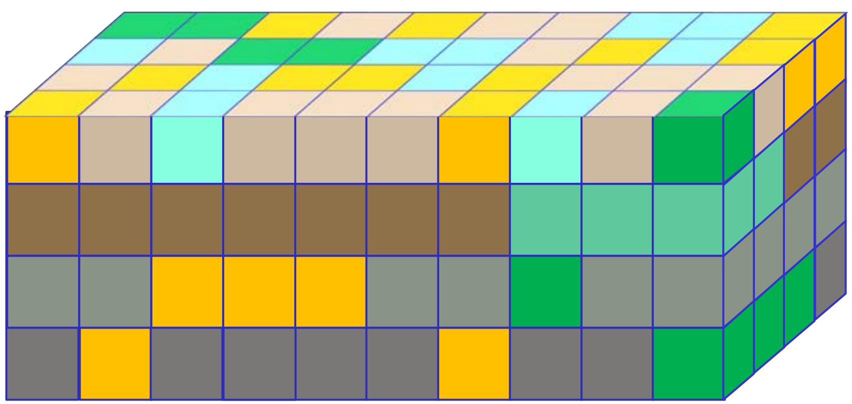
Impact: A “perfect fit” for an observed measurement of 10 feet could be between 9.8 and 10.2 feet within the simulation. Therefore any prediction within the model must be within the “bounds” of this error.

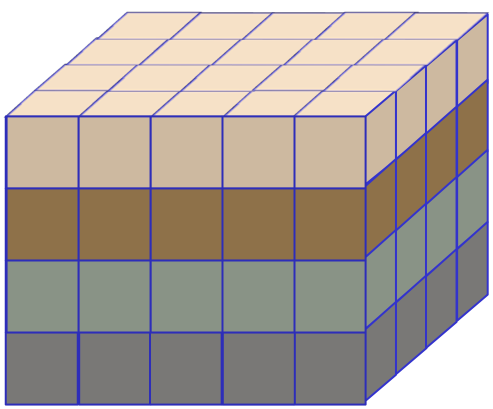
SIMPLE VS. COMPLEX
A TALE OF TWO MODELS

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

$$A + B = C$$

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





WASHINGTON FACILITIES

Two Installations, located within
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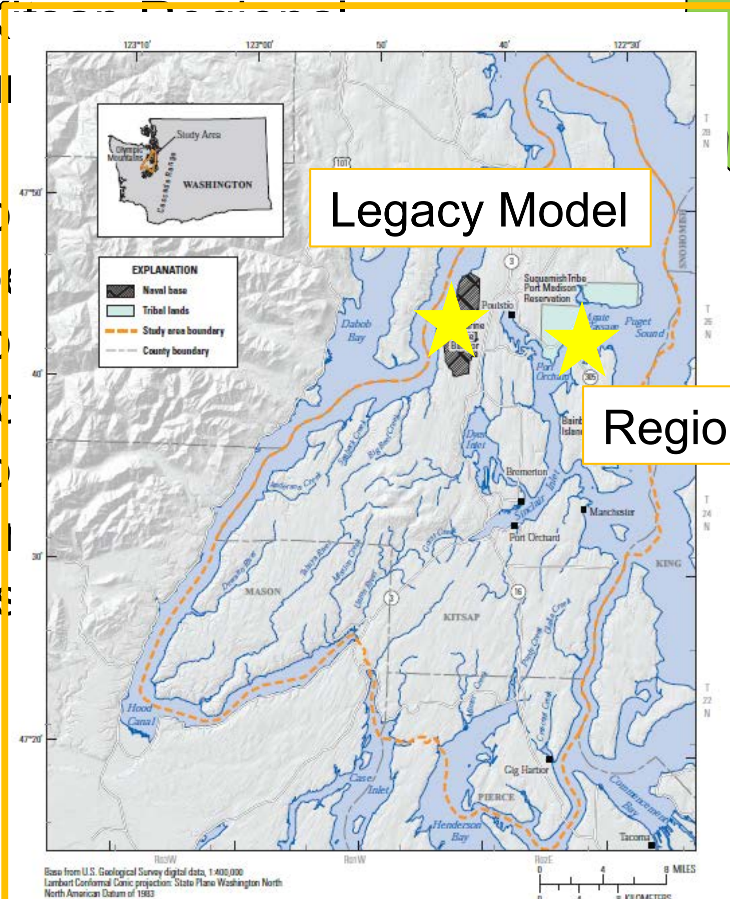
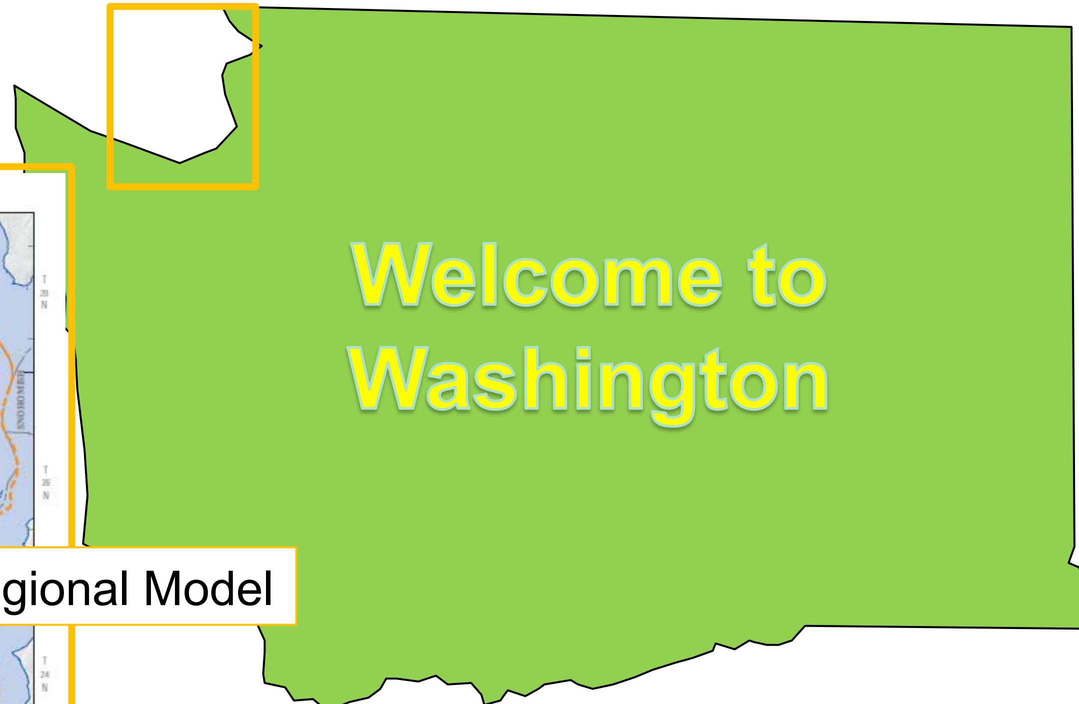


Figure 1. Location of the Kitsap Peninsula study area, west-central Washington.



Via: Welch, 2016 (USGS)

NAVAL BASE KITSAP

When A Simpler Model Would be Best

(even if the site is complex)

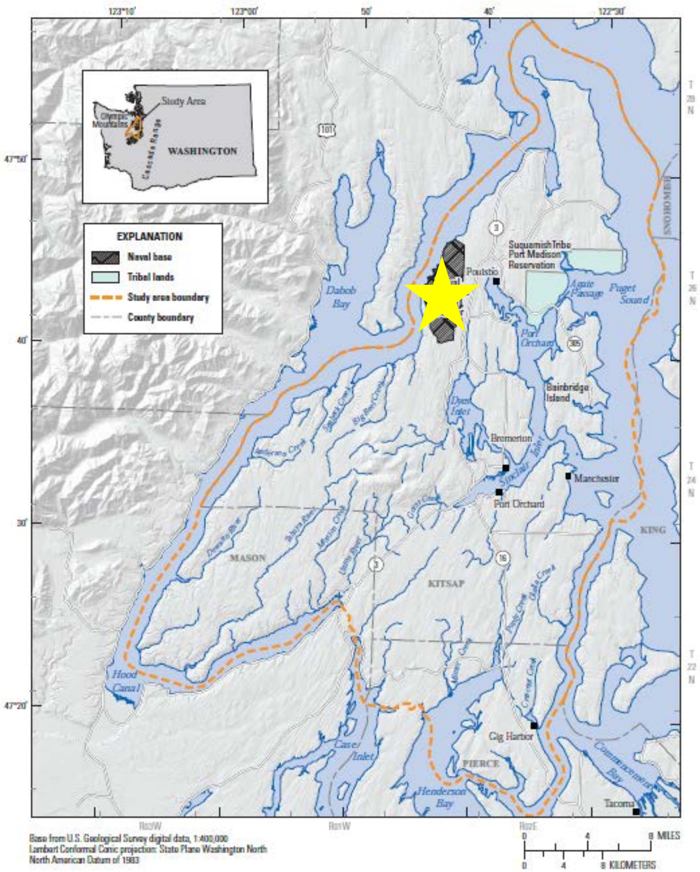
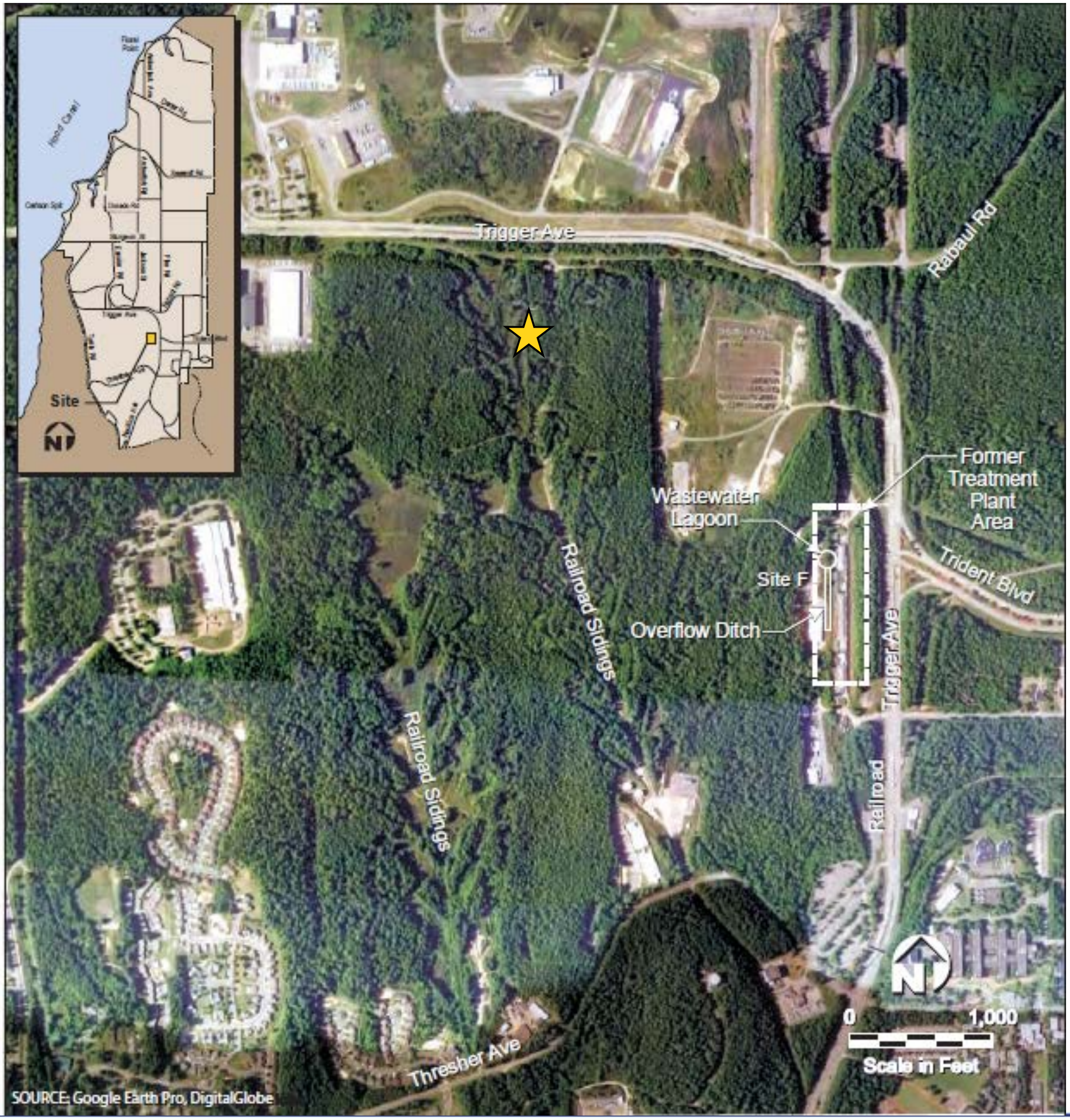


Figure 1. Location of the Kitsap Peninsula study area, west-central Washington.

Via: Welch, 2016 (USGS)

LOCATION OU 2, SITE F



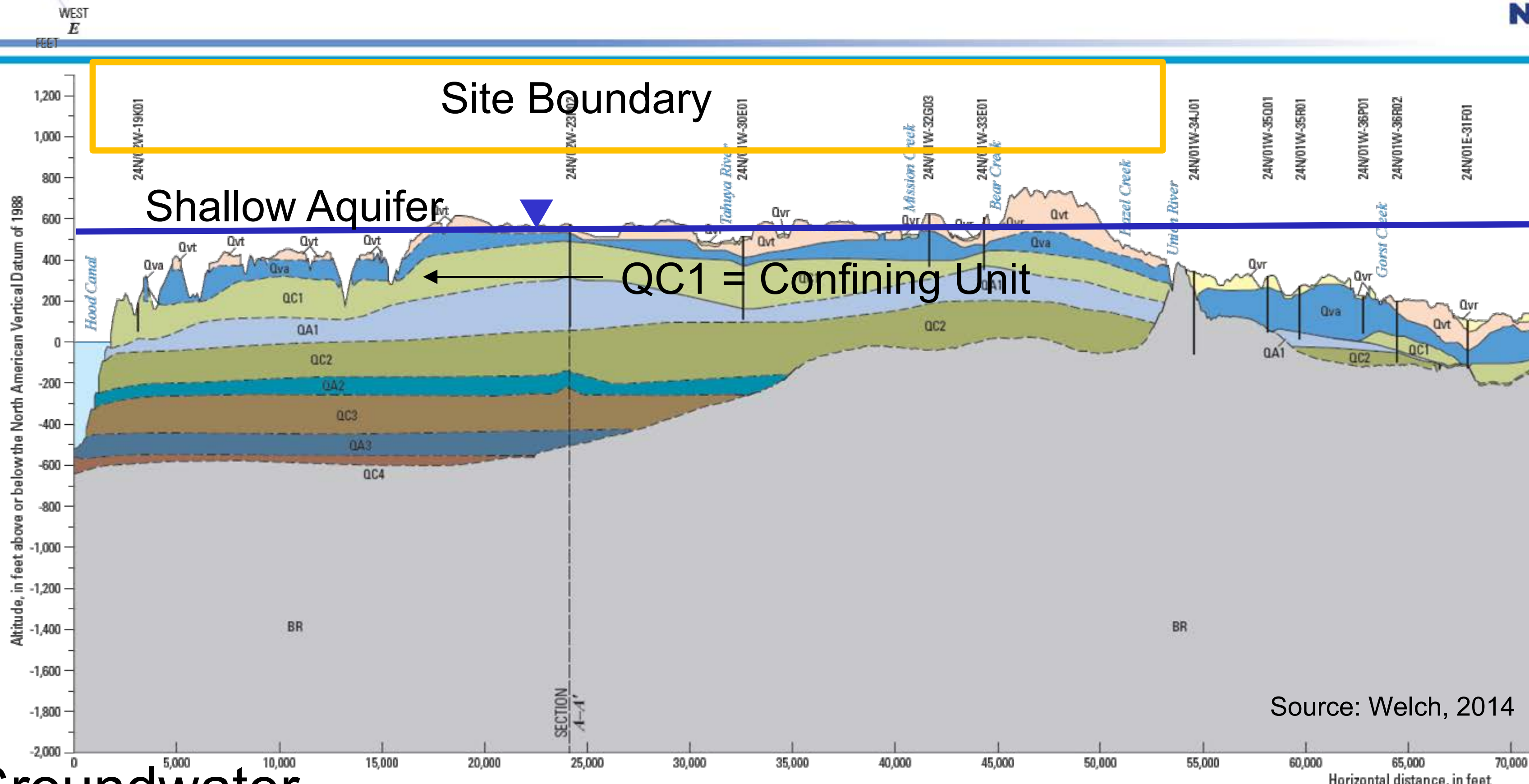
~0.75-acre site

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.

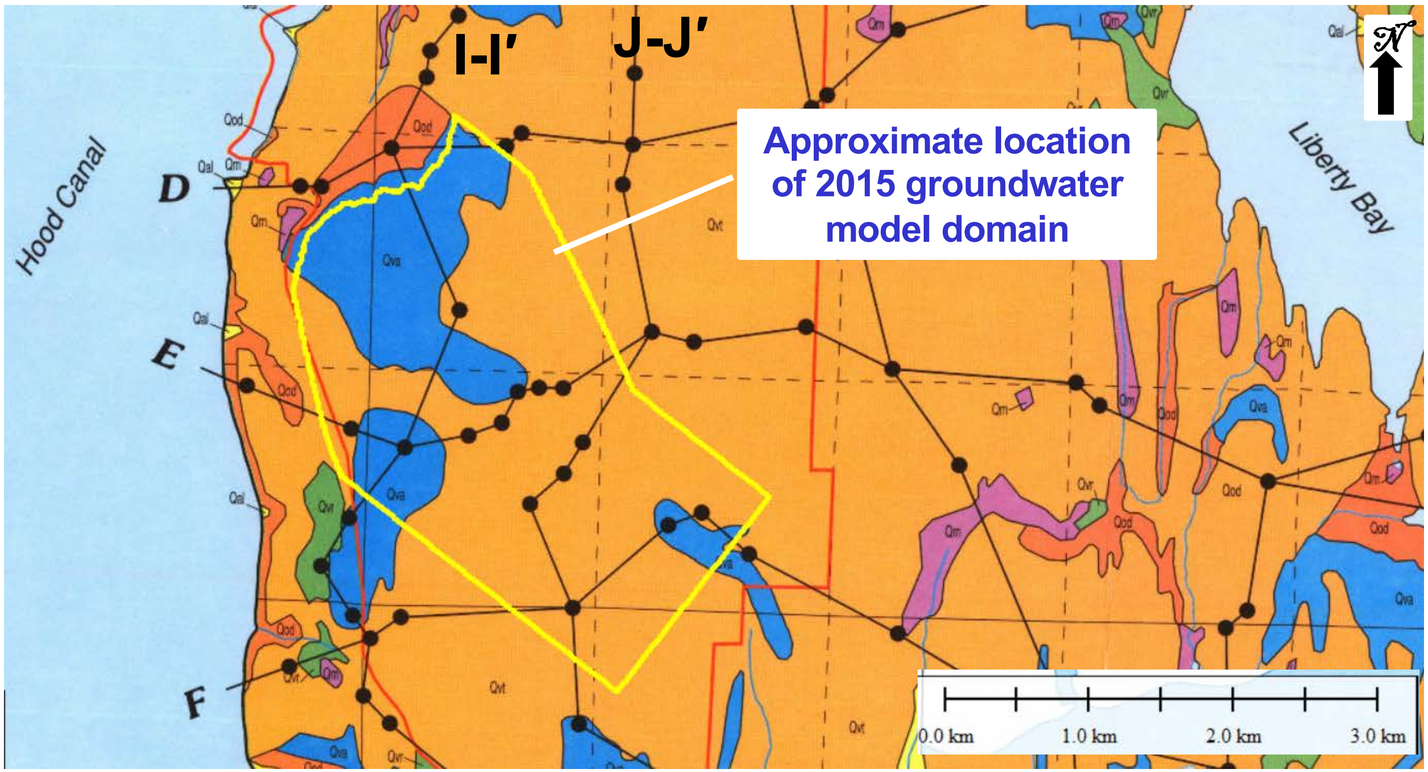
Sea Level Aquifer: Confined by aquitard 80-100 feet below shallow aquifer. Not impacted. Water supply for Vinland.

OU 2 – SITE F HISTORY

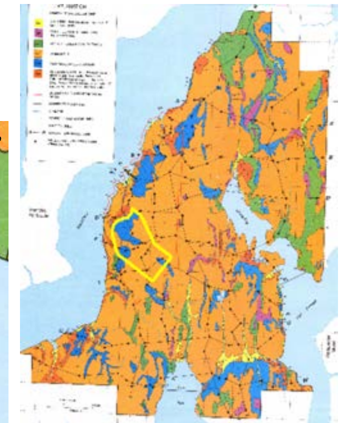
Former Wastewater Location

- 1960-~1972: Unlined lagoon and overflow ditch used for ordnance demilitarization wastewater disposal
  - **Created a subsurface contamination problem**
- 1972: 500 ft^3 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



Modified from : Kahle 1998



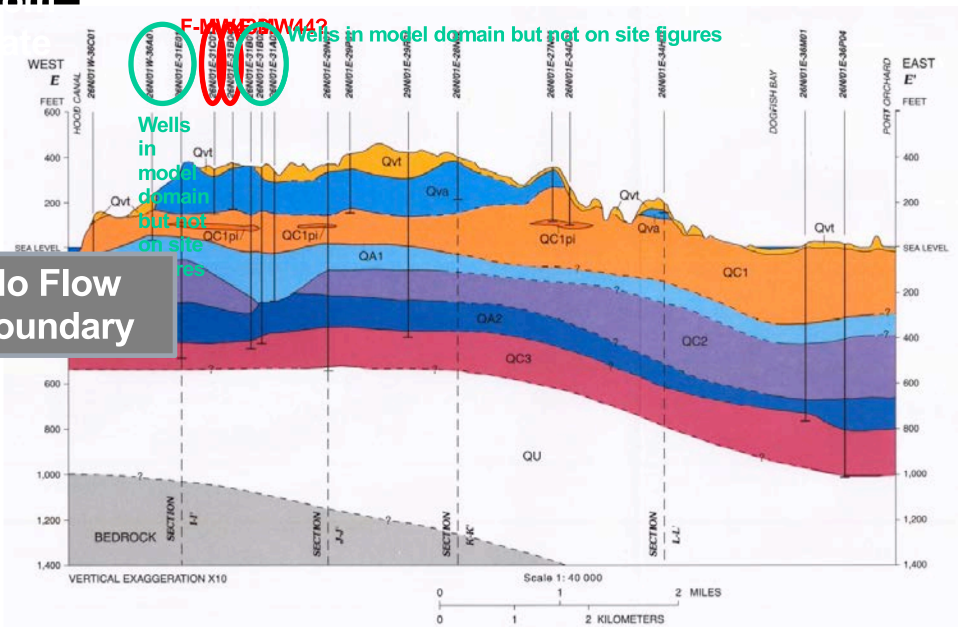
EXPLANATION

GENERALIZED GEOLOGIC UNIT

- Qal — ALLUVIUM - includes stream, beach, and landslide deposits
- Qm — MARSH DEPOSITS - includes bog deposits and peat
- Qvr — VASHON RECESSIONAL 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

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%



No Flow Boundary

General Head Boundary

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

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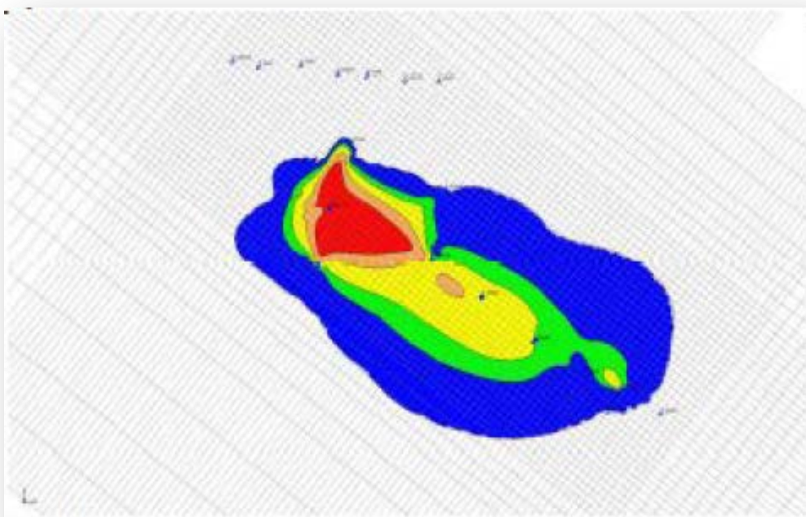
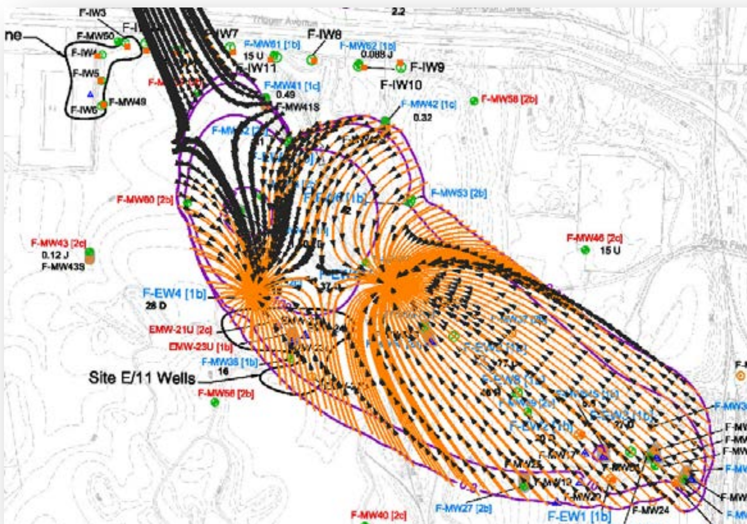
LEGACY MODEL - CONCERNS

- Model fit well, but did not mimic know “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



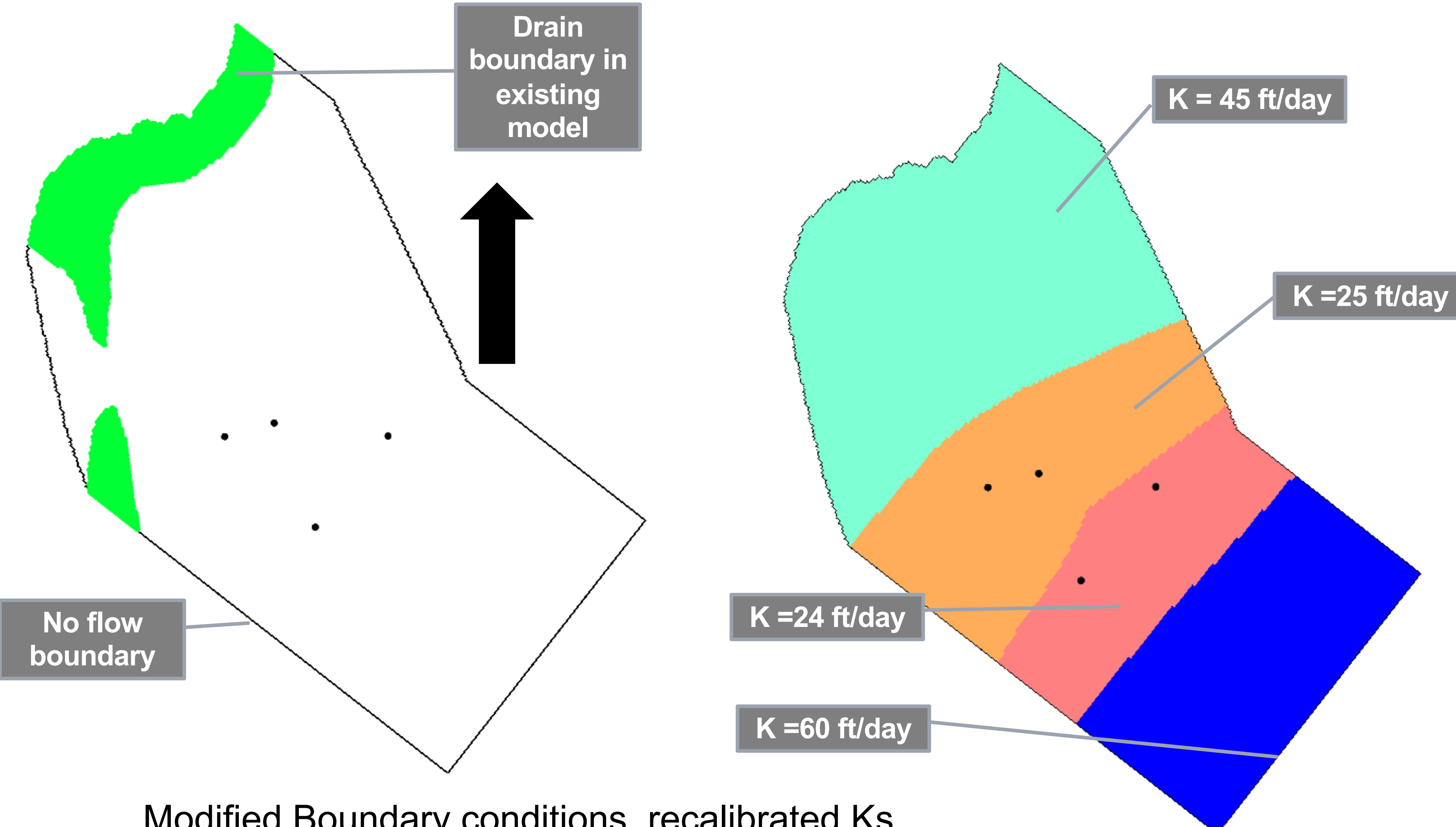
2015 model from USACE 2015

VS



Updated model from SEALASKA (Via GSI) 2018

SIMPLIFIED MODEL UPDATES

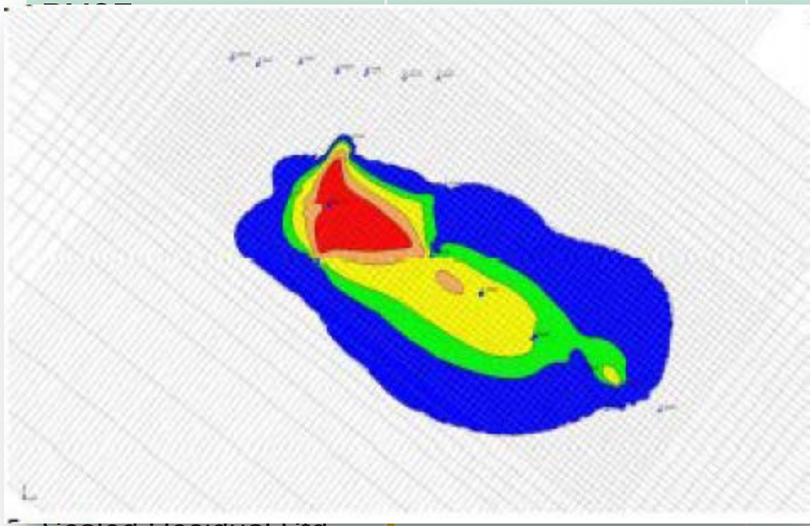


Modified Boundary conditions, recalibrated Ks

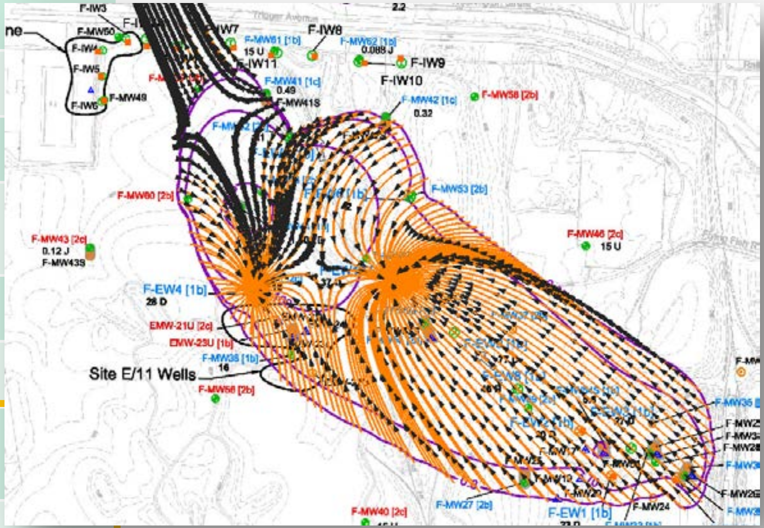
MODEL COMPARISONS

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
RMSE	[illegible]	2.49
[illegible]	[illegible]	-12.75
[illegible]	[illegible]	16.31
[illegible]	[illegible]	6,132
[illegible]	[illegible]	24.07
[illegible]	[illegible]	-2.50%
[illegible]	[illegible]	7.80%
Scaled Residual Std. Dev	4.10%	[illegible]
Scaled RMSE	4.10%	10.40%

RESULT:
more realistic transport with simpler boundary conditions



2015 model from USACE 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

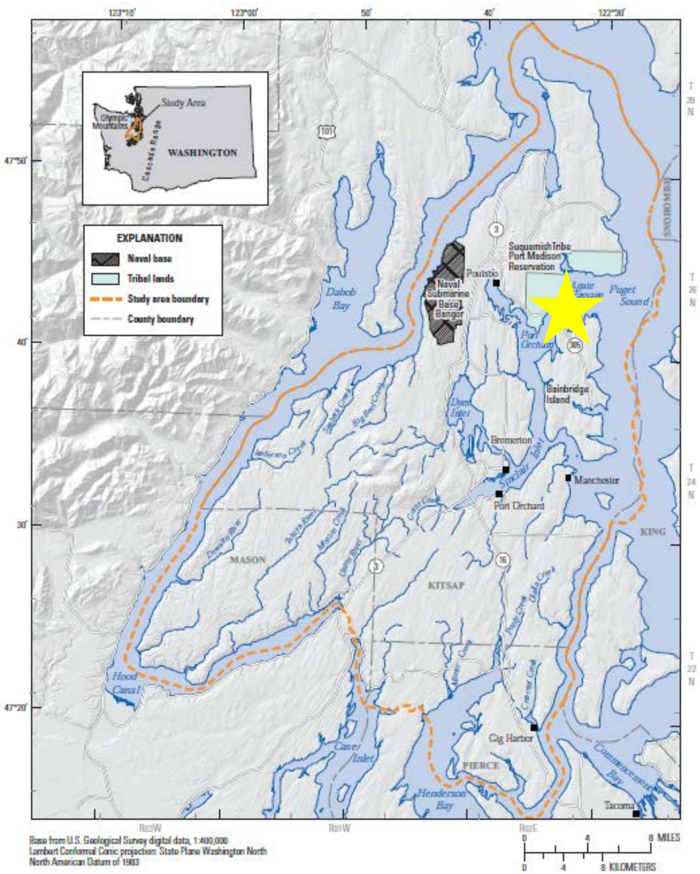


Figure 1. Location of the Kitsap Peninsula study area, west-central Washington.

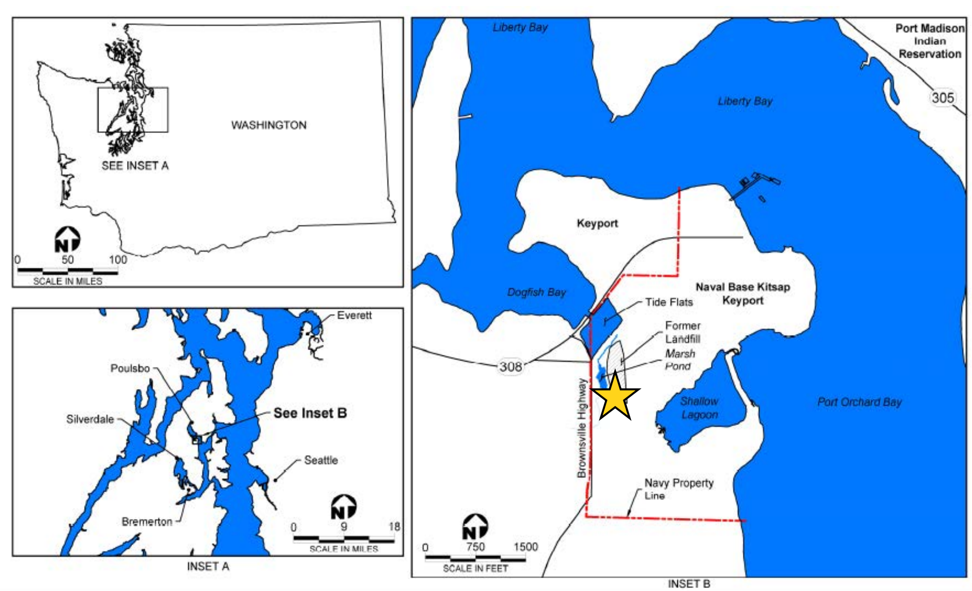
Via: Welch, 2016 (USGS)

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



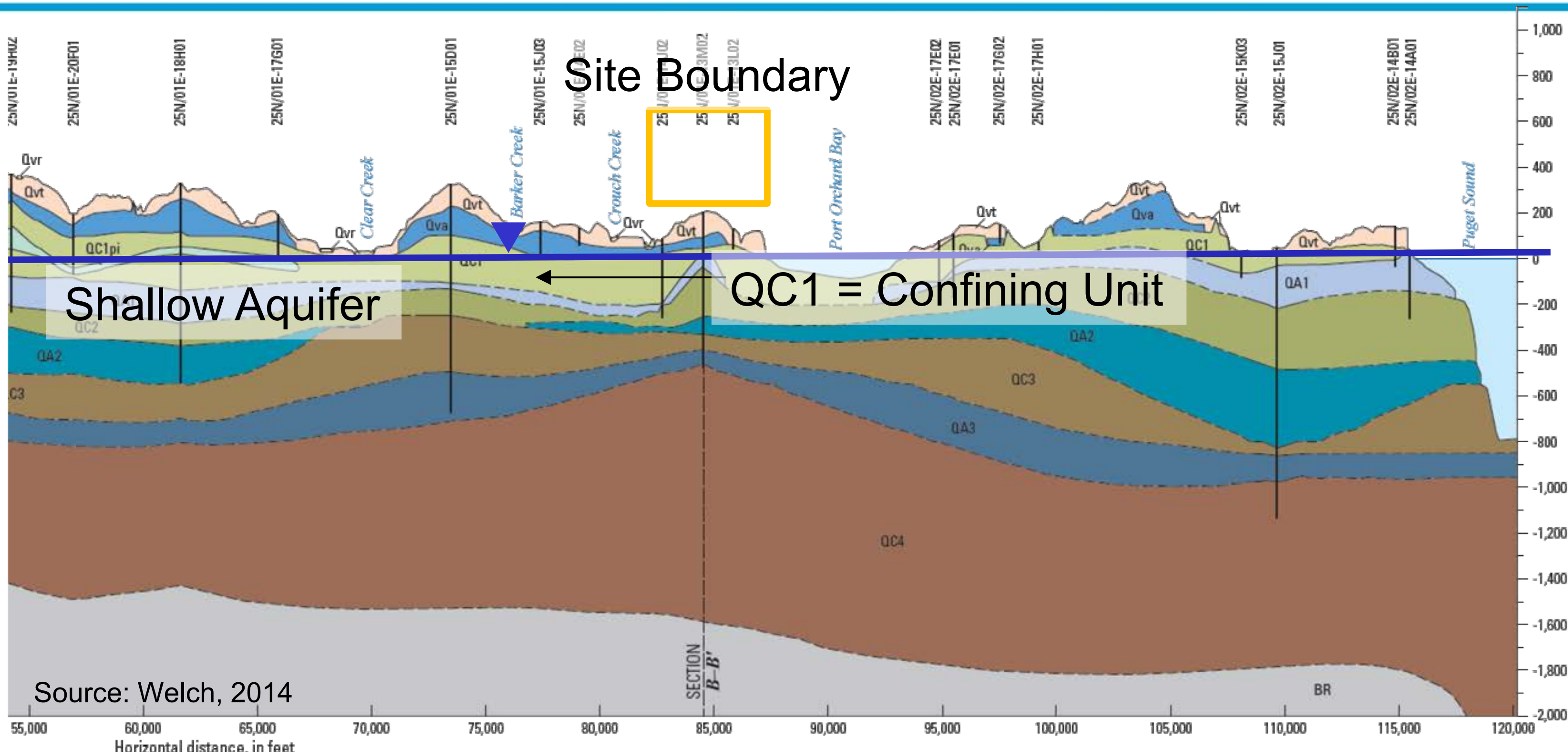
OU 1 – SOUTH PLANTATION HISTORY

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

NAVFAC

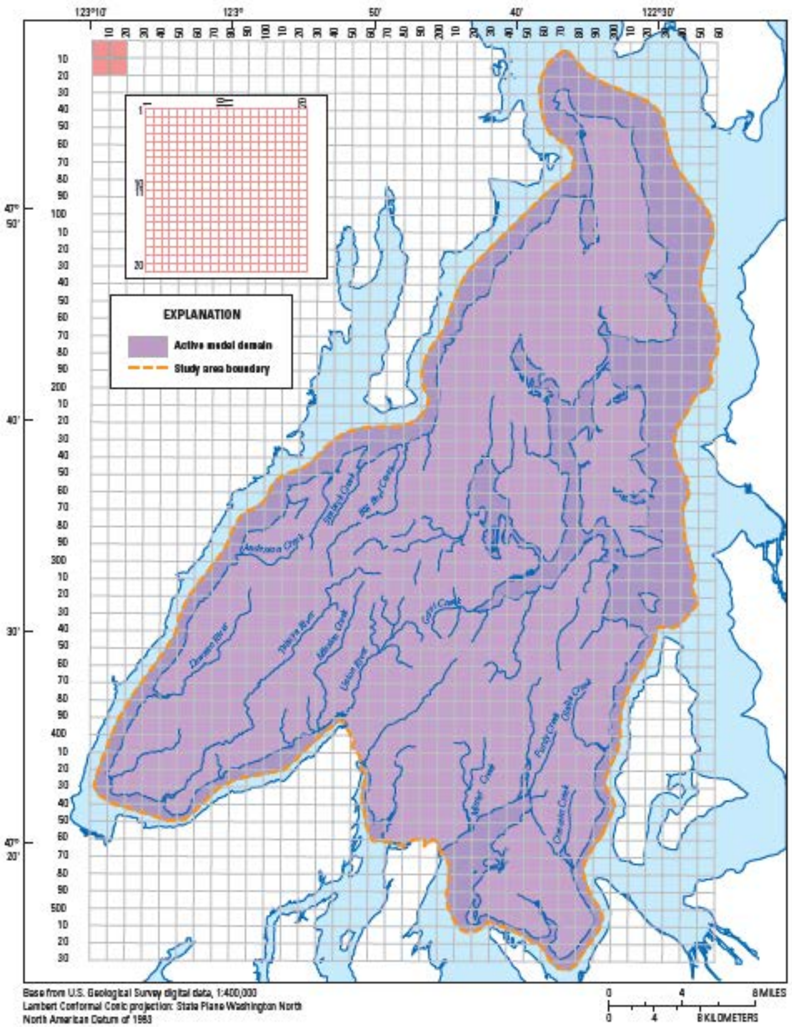


Figure 2. Location and extent of the groundwater model grid, west-central Washington. The insert depicts the detailed horizontal discretization for the first 20 rows and columns of the grid.

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

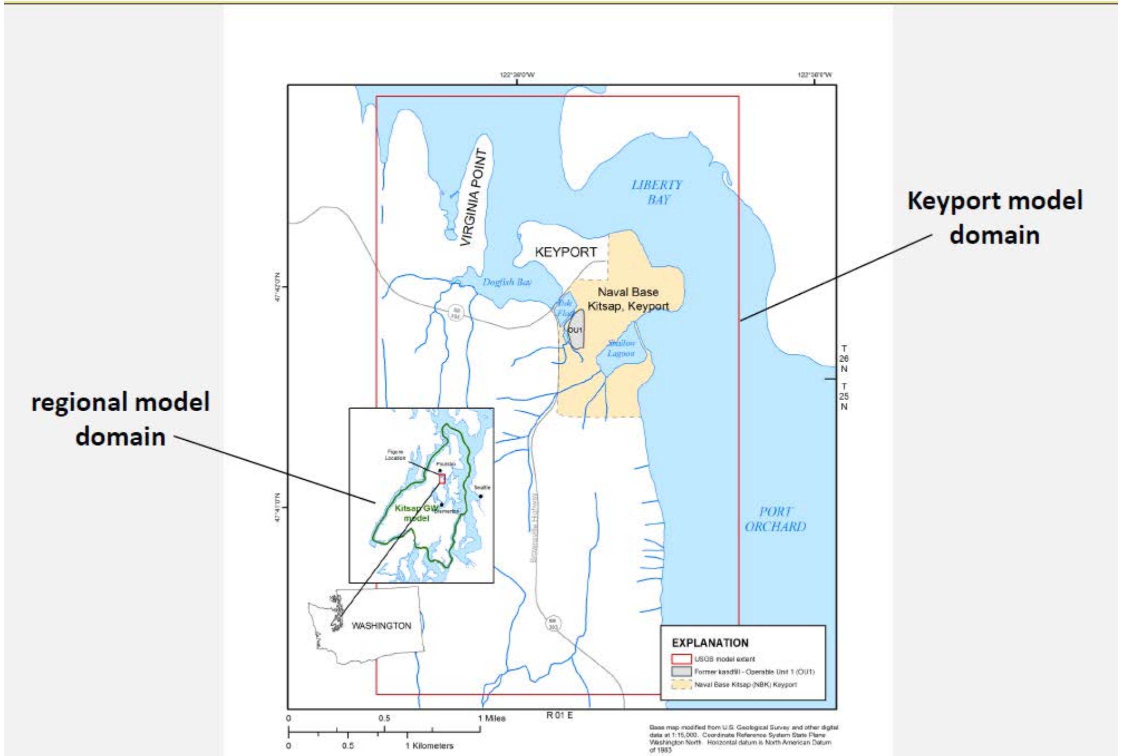
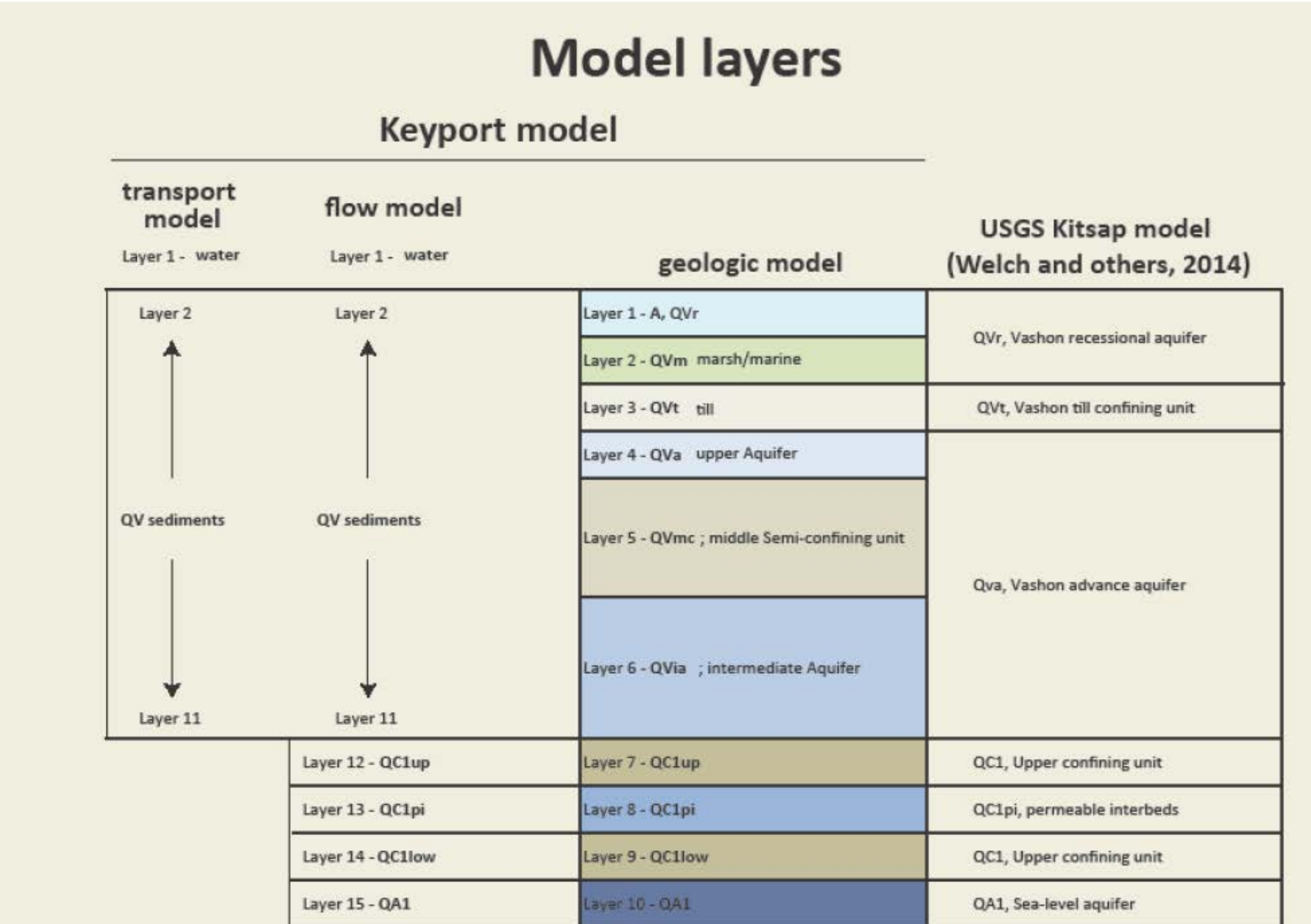


Figure 1. Location of the study area near Operable Unit 1, Naval Base Kitsap (NBK) Keyport in Keyport, Washington

- 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

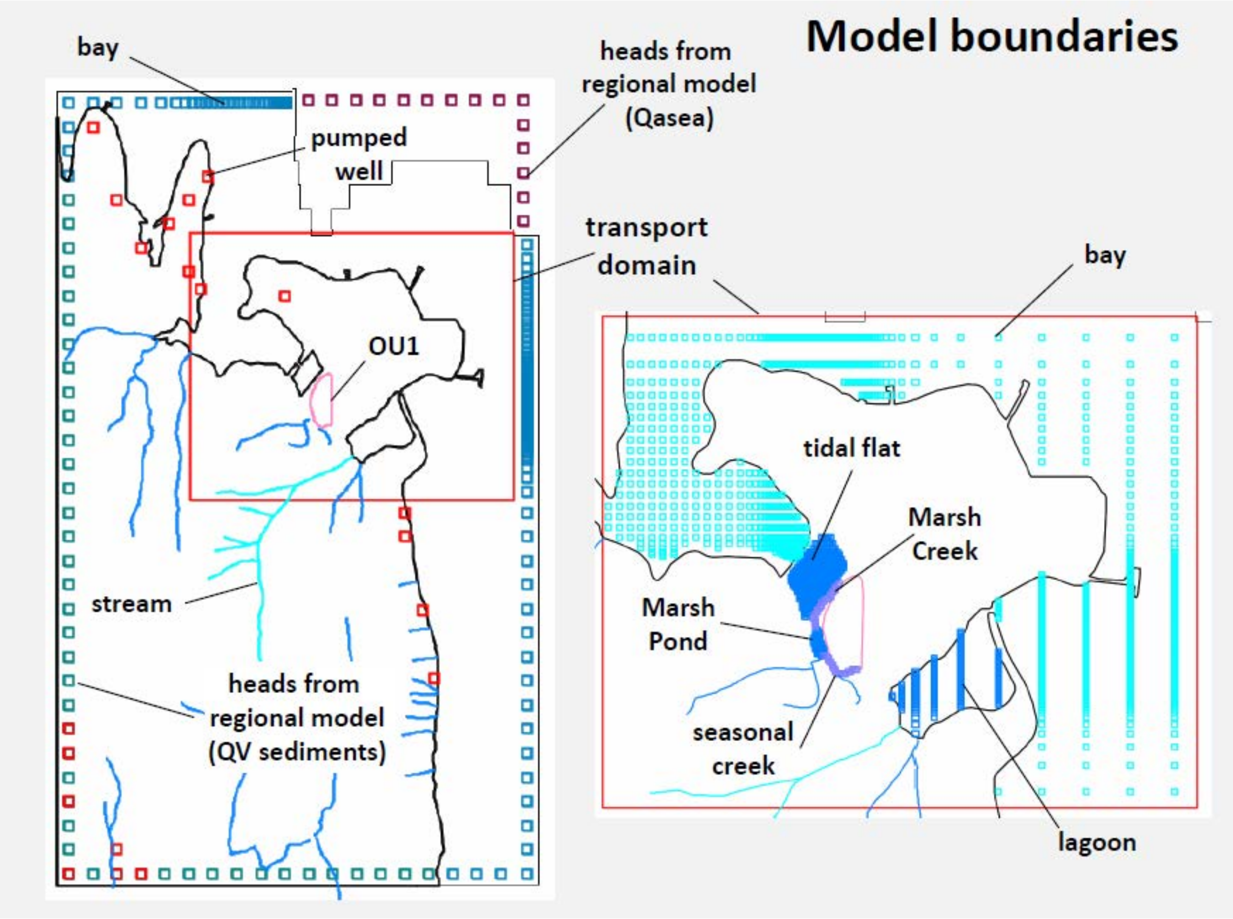
Via: Yager 2019 (USGS, in-development)

VERTICAL REFINEMENT



Via: Yager 2019 (USGS, in-development)

REFINED MODEL DOMAIN



Via: Yeager 2019 (USGS, in-development)

CALIBRATION - CONCERNS

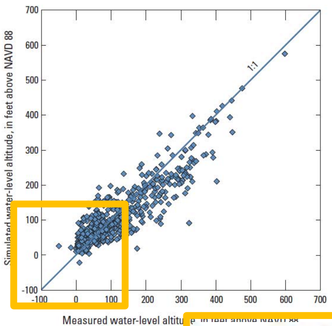
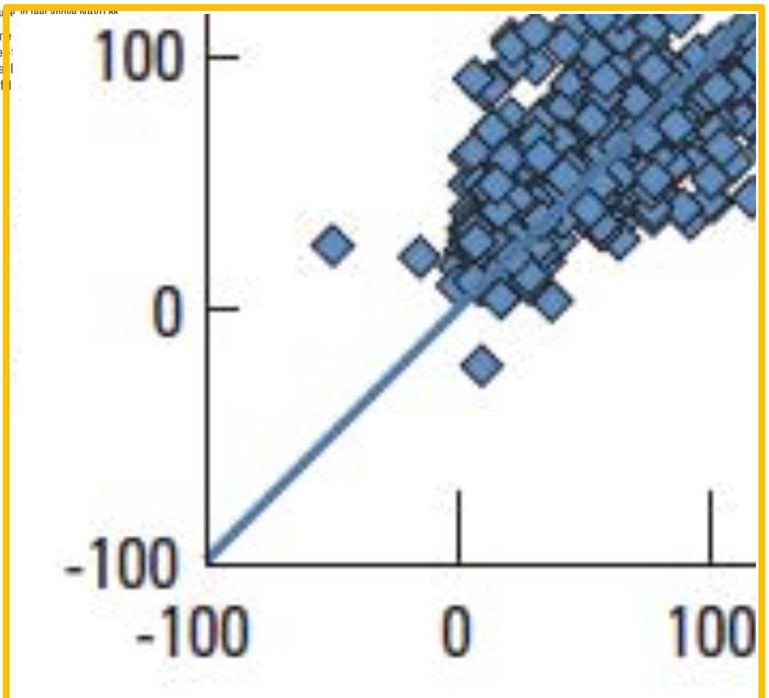
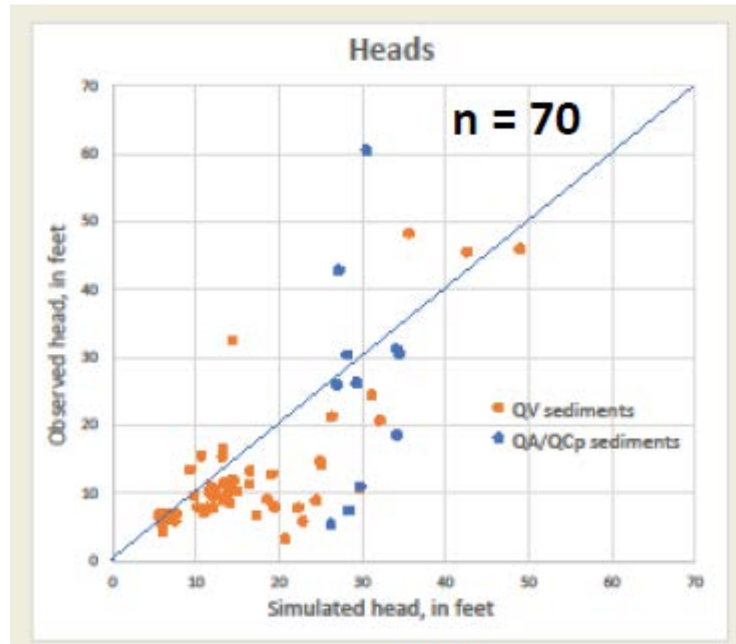


Figure 5. Simulated and m…
altitudes in the groundwate…
Peninsula, west-central Wa…
American Vertical Datum of…



Via: Welch, 2016 (USGS)

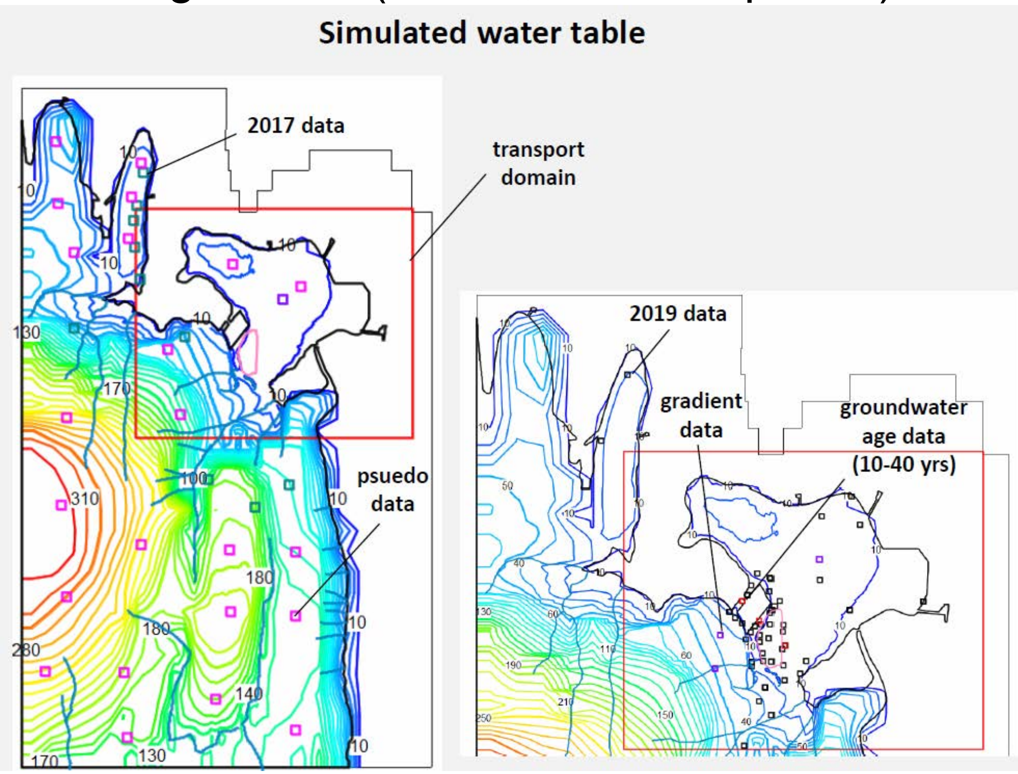
Via: Yager 2019 (USGS, in-development)



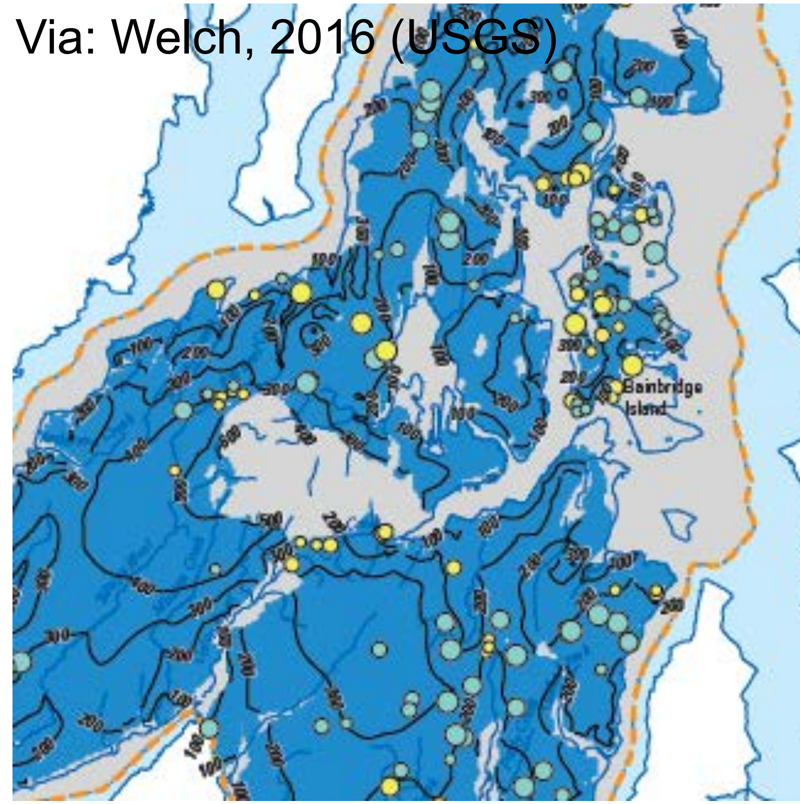
(Still in Final Calibration)
Model Calibration: RMSE at 15%
Average error: 9 ft. (vs. 47 ft.)
Range in heads 60 ft. (vs. 647 ft.)

MODEL COMPARISON – WATER LEVELS

Via: Yager 2019 (USGS, in-development)



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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References

- Frans, Lonna M., and Theresa D. Olsen. *Numerical simulation of the groundwater-flow system of the Kitsap Peninsula, west-central Washington*. No. 2016-5052. US Geological Survey, 2016.
- GSI, 2018, 2019 Presentations to the U.S. Navy. Work- In-Progress
- Hill, Mary C. "The practical use of simplicity in developing ground water models." *Groundwater* 44.6 (2006): 775-781.
- Kahle, S. C. "Hydrogeology of Naval Submarine Base Bangor and Vicinity, Kitsap County, Washington." *Water-Resources Investigations Report* 97 (1998): 4060.
- Lukacs, Paul M., Kenneth P. Burnham, and David R. Anderson. "Model selection bias and Freedman's paradox." *Annals of the Institute of Statistical Mathematics* 62.1 (2010): 117.
- Michaelsen, M., King, A., Gelinas, S. Optimization of an Explosives-Contaminated Groundwater Pump & Treat Remedy Using Bioremediation: Naval Base Kitsap, Bangor Site F. USACE, 2015.
- Welch, Wendy B., Lonna M. Frans, and Theresa D. Olsen. *Hydrogeologic Framework, Groundwater Movement, and Water Budget of the Kitsap Peninsula, West-Central Washington*. No. 2014-5106. US Geological Survey, 2014.
- Yager, R. "Groundwater flow and contaminant transport of the Keyport Peninsula" Presented to the U.S. Navy April 9, 2019. Work-In-Progress