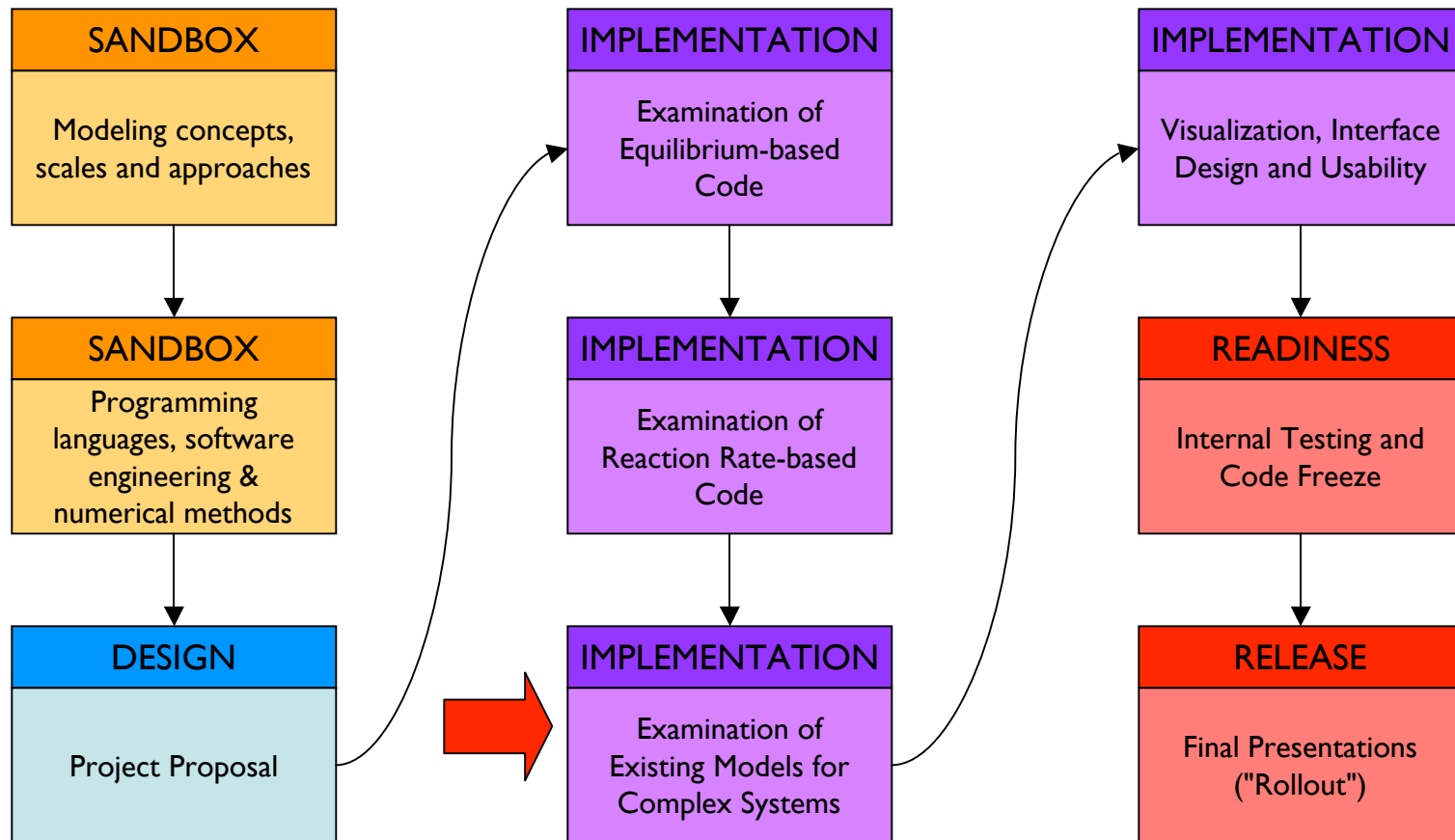


A hand is holding a small, translucent, yellowish, star-shaped object, possibly a piece of coral or a biological specimen, against a background of a beach and ocean. The object has several sharp, pointed edges and a central body. The background shows a sandy beach in the foreground, a calm ocean with gentle waves in the middle ground, and a clear blue sky in the background. The overall scene is bright and sunny.

Modeling Complex Systems

CEE 373

Roadmap



MODELING COMPLEX SYSTEMS

OBJECTIVES

1. To learn how to approach and treat complexity.
2. To learn to critically evaluate models and model output.
3. To examine application of HYDRAQL to complex systems.

MODELING COMPLEX SYSTEMS

1. Approach
2. Validation and verification.
3. Sensitivity analysis.
4. Interpretation.
5. Reporting.

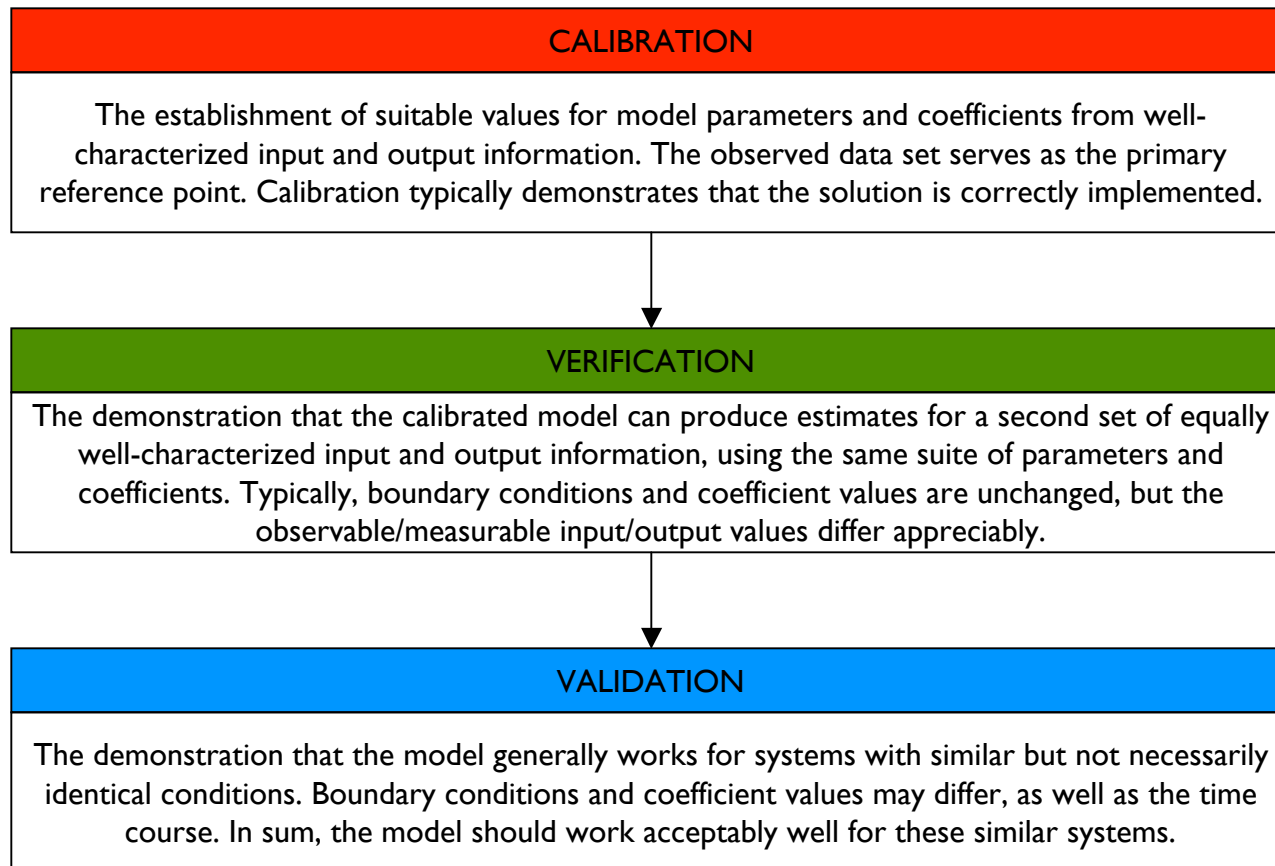
Approach

PUTTING A PLAN TOGETHER

- Get a feel for the accuracy and precision of the observed/measured data.
 - Can you critically assess the analytical methodology used to obtain the data set?
 - Do you have total elemental or speciated analyses?
 - Are you familiar with the conditions during sampling?
 - Could the sample have changed character between sampling and analysis?
 - Is data averaged to reflect multiple sample sets?
- Pull together information/data from secondary sources that may help.
 - Look for documentation of other relevant data.
 - For example, a lab notebook might contain data that was not included in a report/publication.
 - For example, sub-surface properties may be obtained from previous studies.
- Select the model best for your application.
 - Technical merit might not be the primary criteria.
 - Selection might be affected by resource limitations.
- Establish how you are going to decide "goodness of fit."
- Do some trial runs and establish how you will sequence subsequent runs and manage data.

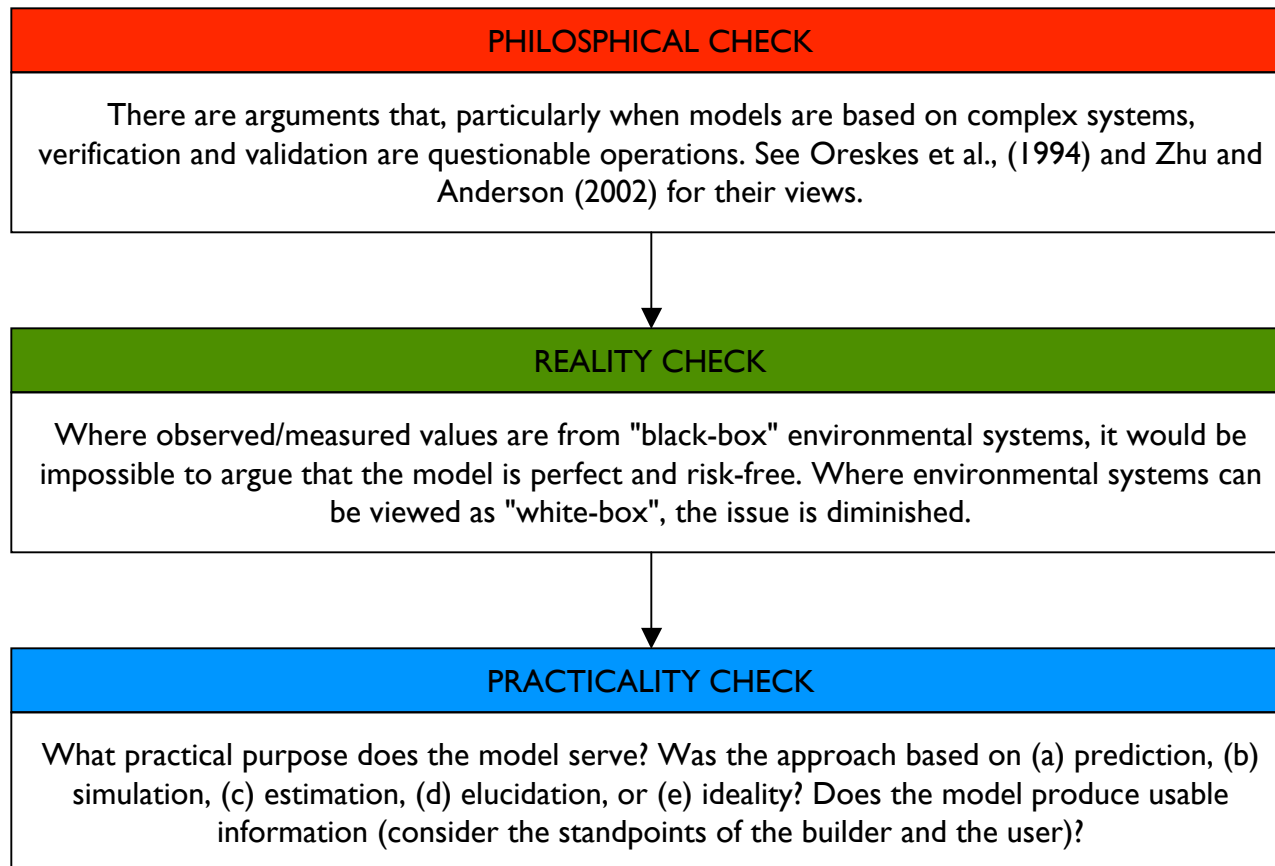
Validation and Verification

THE IDEALITY TEST DRIVE



Validation and Verification

THE REALITY TEST DRIVE



Sensitivity Analysis

PRE-FLIGHT CHECK

- A sensitivity analysis is the process of varying model input parameters over a reasonable range (range of uncertainty in values of model parameters) and observing the relative change in model response.
- The purpose of the sensitivity analysis is to demonstrate the sensitivity of the model simulations to uncertainty in values of model input data.
- The sensitivity of one model parameter relative to other parameters is also demonstrated.
- Sensitivity analyses are also beneficial in determining the direction of future data collection activities. Data for which the model is relatively sensitive would require future characterization, as opposed to data for which the model is relatively insensitive. Model-insensitive data would not require further field characterization. If data are determined to be insensitive to variations in model input parameters, the modeler should assess the possible reasons for this insensitivity.

Interpretation

HOW DO YOU MAKE SENSE OF IT ALL?

REVIEW OF LIMITATIONS & CONSTRAINTS

Check that your application of the model was correct and thorough. Look for incorrect assumptions or data entry mistakes, To what extent did the model allow you to describe and consider boundary conditions and constraints?



DEALING WITH UNCERTAINTY

Aspects of uncertainty in modeling is discussed by Bethke (1996). A source of error evaluation is warranted and a discussion of any issues is critical to reporting.



CLOSURE AND SPECULATION

Given the uncertainties from the modeling, one can proceed by methodically bringing closure to the issues by "scrubbing" the information. Distinguish showstopper issues from issues which can be argued to have little or no effect on the conclusions. Speculation is common, but should be clearly couched as such and well-supported.

Interpretation

BETHKE'S DISCUSSION OF UNCERTAINTY

- Is the chemical analysis used sufficiently accurate to support the modeling study?
- Does the thermodynamic dataset contain the species and minerals likely to be important in the study?
- Are the equilibrium constants for the important reactions in the thermodynamic dataset adequately accurate?
- Can the species' activity coefficients be calculated accurately?
- Do the kinetic rate constants and rate laws apply well to the system being studied?
- Is the assumed nature of equilibrium appropriate?
- Most importantly, has the modeler conceptualized the reaction process correctly?

ZHU & ANDERSON'S VERSION

- Is the chemical analysis used sufficiently accurate to support the modeling study?
- Does the thermodynamic database in the program contain the aqueous species, surface complexes, and minerals likely to be important in the solution?
- Are the equilibrium constants for the important reactions in the thermodynamic database sufficiently accurate to warrant the conclusions?
- Is the ionic strength small enough so that the activity coefficient model in the modeling code is applicable?

In general, check that the model did not venture further than the intended scope. Charge balance, mass balance and activity coefficient model limits are typically necessary.

Reporting

COMMUNICATING YOUR FINDINGS

- Reproducibility
- Clarity
- Traceability
- Critical self-assessment
- Statement of all assumptions and constraints
- Further studies

Case Studies

- Hydrosalinity model
 - Modeling Transient Root Zone Salinity
 - Conceptual Irrigation Return Flow Hydrosalinity Model
 - Code and Calibration/Verification Data
- Nonreversible Adsorption of Divalent Metal Ions (Mn^{II} , Co^{II} , Ni^{II} , Cu^{II} , and Pb^{II}) onto Goethite: Effects of Acidification, Fe^{II} Addition, and Picolinic Acid Addition
 - Interpreting and refining model data using the minimization of the sum of the square of the residuals
- Surface and Solution Speciation of Ag^{I} in a Heterogeneous Ferrihydrite-Solution System with Thiosulfate
 - Example of interpretation and reporting
 - Lab exercise to reproduce model data