IMPROVE Quality Assurance Assessment

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IMPROVE Steering Committee Meeting
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IMPROVE QA System Assessment

- Data management system needs major overhaul to address key QA problems
  - Robust archival system for key dataset stages
  - Tracking of changes to data and data processing
  - Data reproducibility
  - Minimization of manual data entry
  - Ready access to routine, special study, and quality control data

IMPROVE QA System Assessment

- Guidance and documentation
  - Quality Assurance Project Plan (QAPP)
  - Standard operating procedures (SOPs)
  - Metadata
- Data validation
  - Objective data quality standards
  - Short- versus long-term view
- Quality control data
  - Historic data
  - Determine adequacy of current QC data collection
- Internal and external audits

QAPP and SOPs

- QAPP was written in 2002
  - Needs major revision
  - Requires steering committee decisions on measurement and data quality objectives (MQO/DQOs)
- SOPs were written in 1996 -1997
  - Need updating to reflect current procedures
  - No copper XRF SOP
  - Many procedures are in transition currently and several SOPs will require complete overhaul
- QAPP and SOPs need to be revised by end of 2006

Metadata History and Updates

- Site history and location metadata holdings at CNL were delivered to CIRA and added to the CIRA database
  - 9800 site history records added to the CIRA database for all currently operational sites for 1988-2004
- History updates for 1988-2004 are being compiled for XRF, PIXE, and PESA analyses
- Semi-annual metadata updates will be delivered to CIRA

Site History Metadata Example

Site History

History	ChangeType	ChangeDate	Description
ACAD1	Operational	09/11/2002	Routine annual maintenance
ACAD1	Operational	08/29/2003	A1 Module Flow Calibration
ACAD1	Operational	08/29/2003	B1 Module Flow Calibration
ACAD1	Operational	08/29/2003	C1 Module Flow Calibration
ACAD1	Operational	08/29/2003	C1 Module pump replaced
ACAD1	Operational	08/29/2003	D1 Module Flow Calibration
ACAD1	Operational	08/29/2003	D1 Module pump replaced
ACAD1	Operational	08/29/2003	Routine annual maintenance
ACAD1	Operational	12/19/2003	Sampler controller replaced
ACAD1	Operational	02/11/2004	Ice on Module D1 filter cartridge, used heat gun to free up
ACAD1	Operational	02/14/2004	Ice on Module D1 filter cartridge, used heat gun to free up
ACAD1	Operational	04/02/2004	A1 Module pump Replaced
ACAD1	Operational	05/04/2004	B1 Module electronic box replaced
ACAD1	Operational	05/07/2004	A1 Module Electronic Box replaced
ACAD1	Operational	07/08/2004	A1 Module Electronic Box replaced
ACAD1	Operational	07/24/2004	A1 Module Flow Calibration
ACAD1	Operational	07/24/2004	B1 Module Flow Calibration
ACAD1	Operational	07/24/2004	C1 Module Flow Calibration
ACAD1	Operational	07/24/2004	D1 Module Flow Calibration
ACAD1	Operational	07/24/2004	Photos Taken
ACAD1	Operational	07/24/2004	Routine annual maintenance
ACAD1	Operational	02/08/2005	B1 Module pump replaced
ACAD1	Operational	04/05/2005	B1 Module pump replaced

New CIRA Integrity and Validation Checks

- New data integrity tests were implemented to address data reporting problems
  - Consistency between flags and data values
  - Exclusion of internal CNL flags in data deliveries
  - Data record completeness (e.g., mdl & unc with each data value)
  - Delivery file completeness
- Data validation checks were expanded to add objectivity and breadth to the visual inspection
  - Al, Ca, Si, and Ti are examined individually and in relation to Fe and “average crustal rock”
  - Nitrate is examined individually and in relation to reconstructed fine mass
  - Z-scores for SO_4 and S used to determine what percentage of the dataset agrees within measurement uncertainty

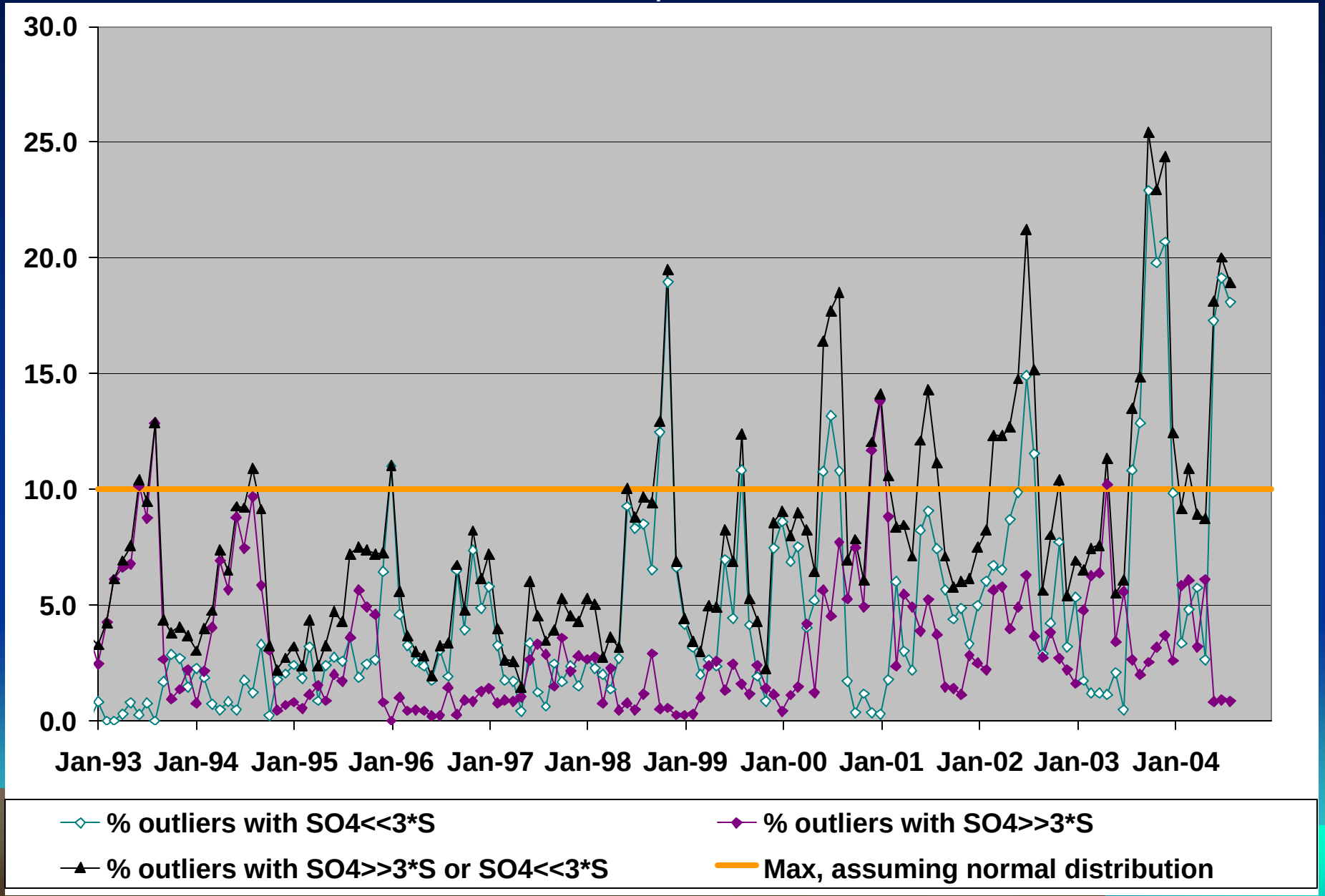
CIRA Historical Review and Quarterly Data Validation Reports

- The data validation process includes analysis of all major parameters including:
  - Sulfate
  - Carbon
  - Nitrate
  - Individual soil elements
  - Particle cut point
  - Mass closure
- Reviewed data from 1988-2003.
  - Report will be posted on the web and included in the next IMPROVE report.
- Starting with 2004 data, each data delivery has undergone secondary data validation at CIRA.
  - Quarterly reports will be posted on the web.

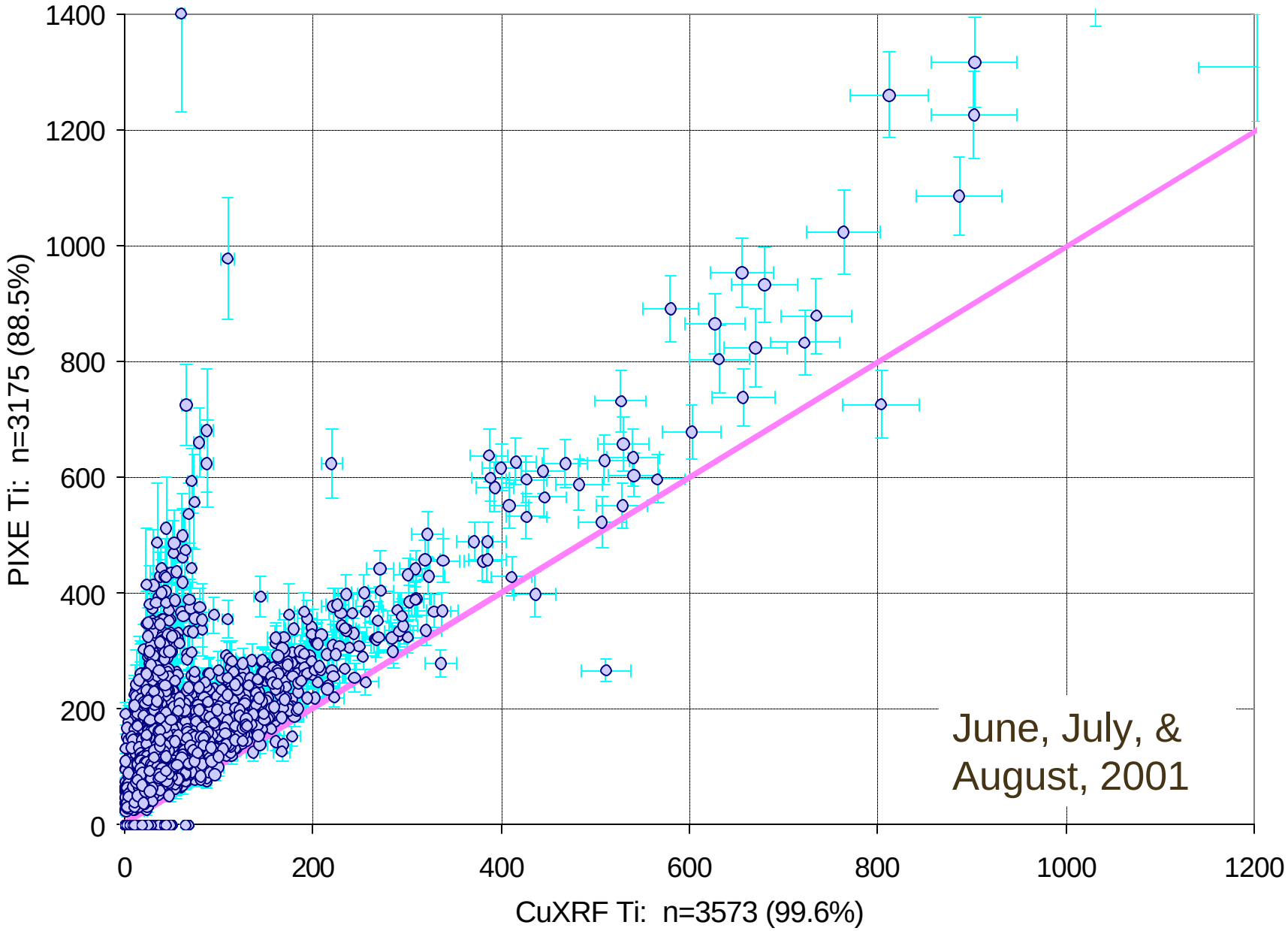
Historical Review: Key Problems Identified

- SO_4 to S comparability has degraded in recent years
- Al not reliably detected, both with PIXE and XRF
- Ti contamination issue with PIXE
- Persistent flow problems at several sites
- Severe data quality problems at CHAS, SWAN and MING
  - Data removed from CIRA database

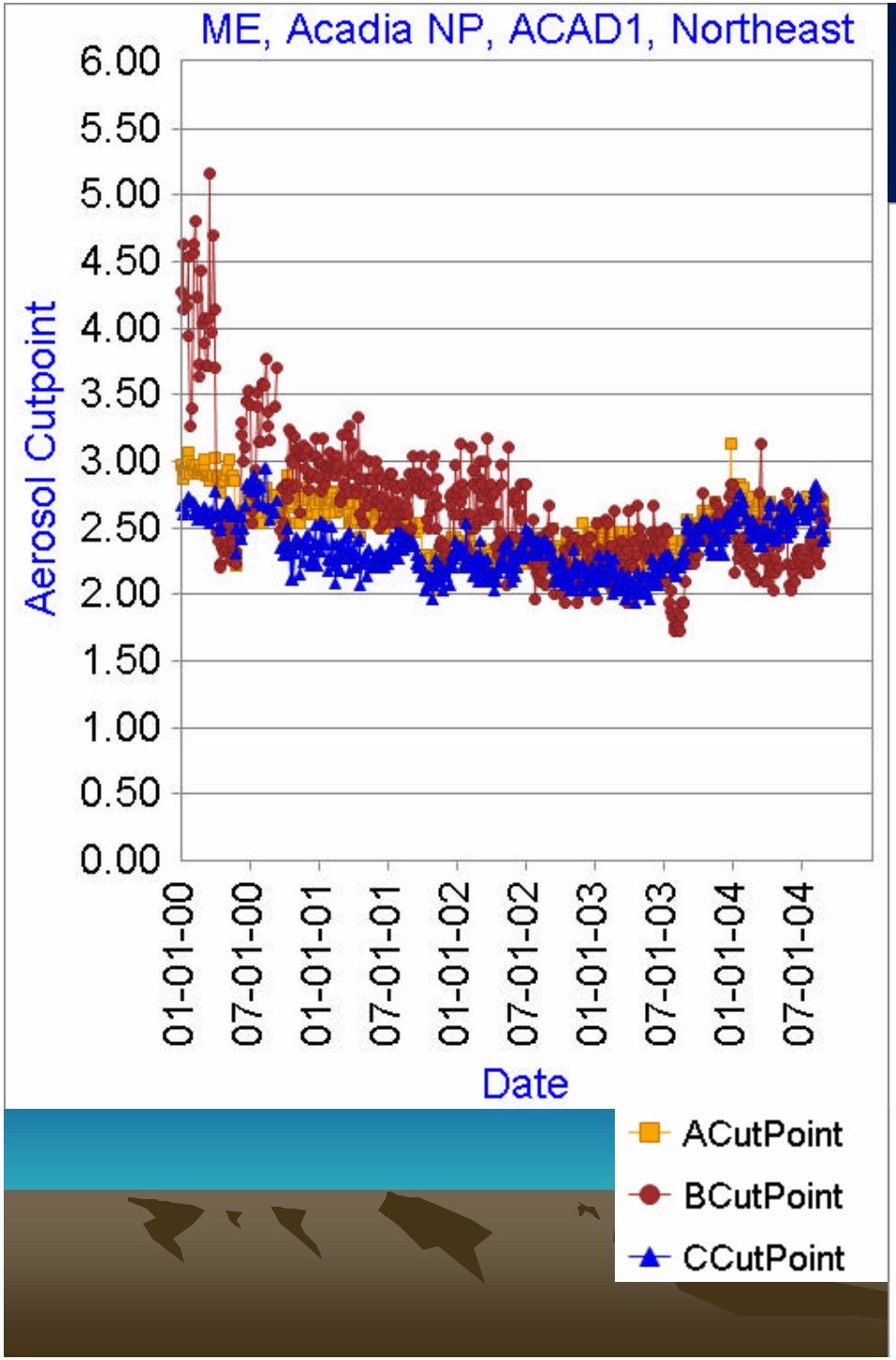
Percent of valid sample pairs with significant disagreement between SO_4 and 3*Sulfur

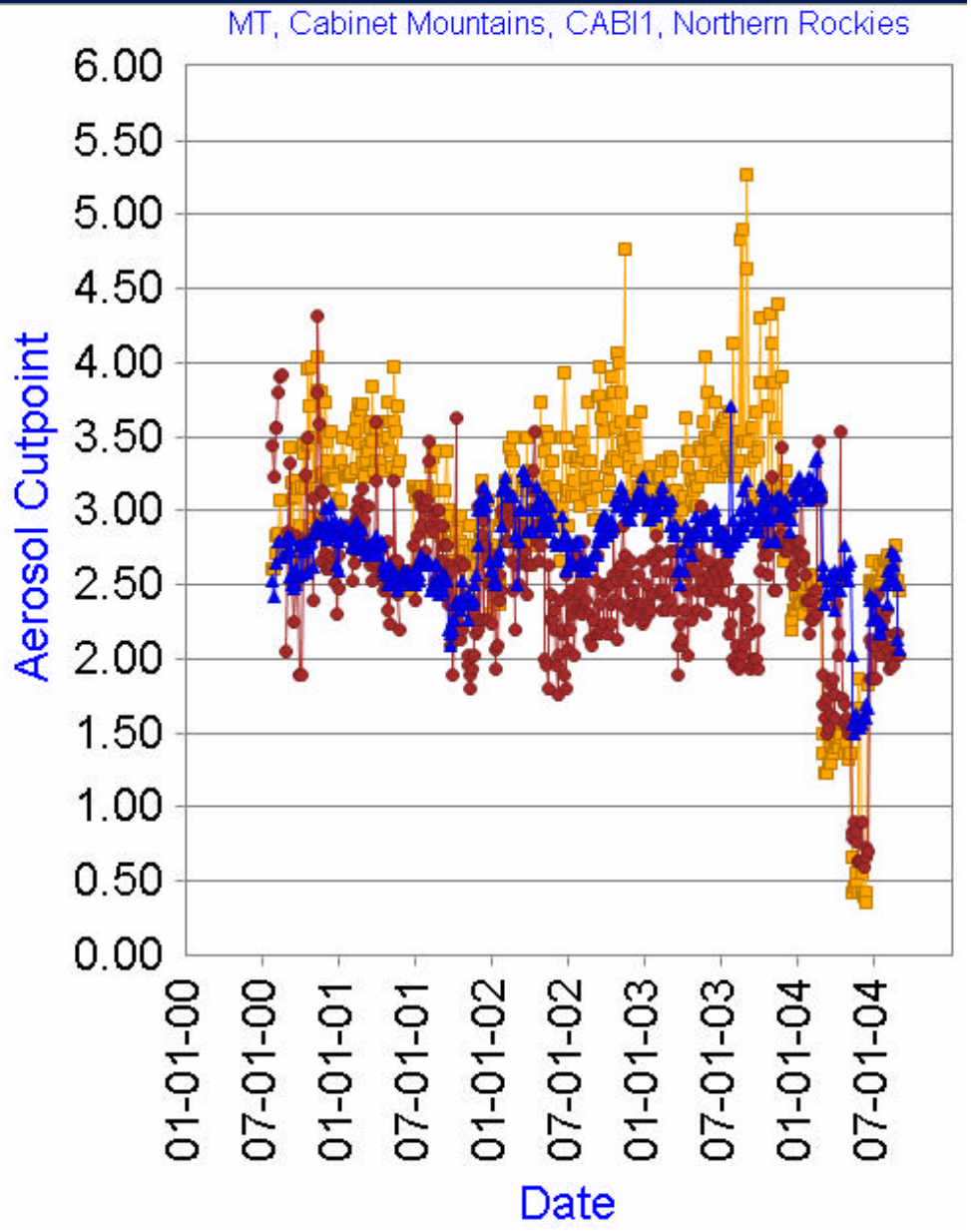


Ti Interference from Slide Mount?

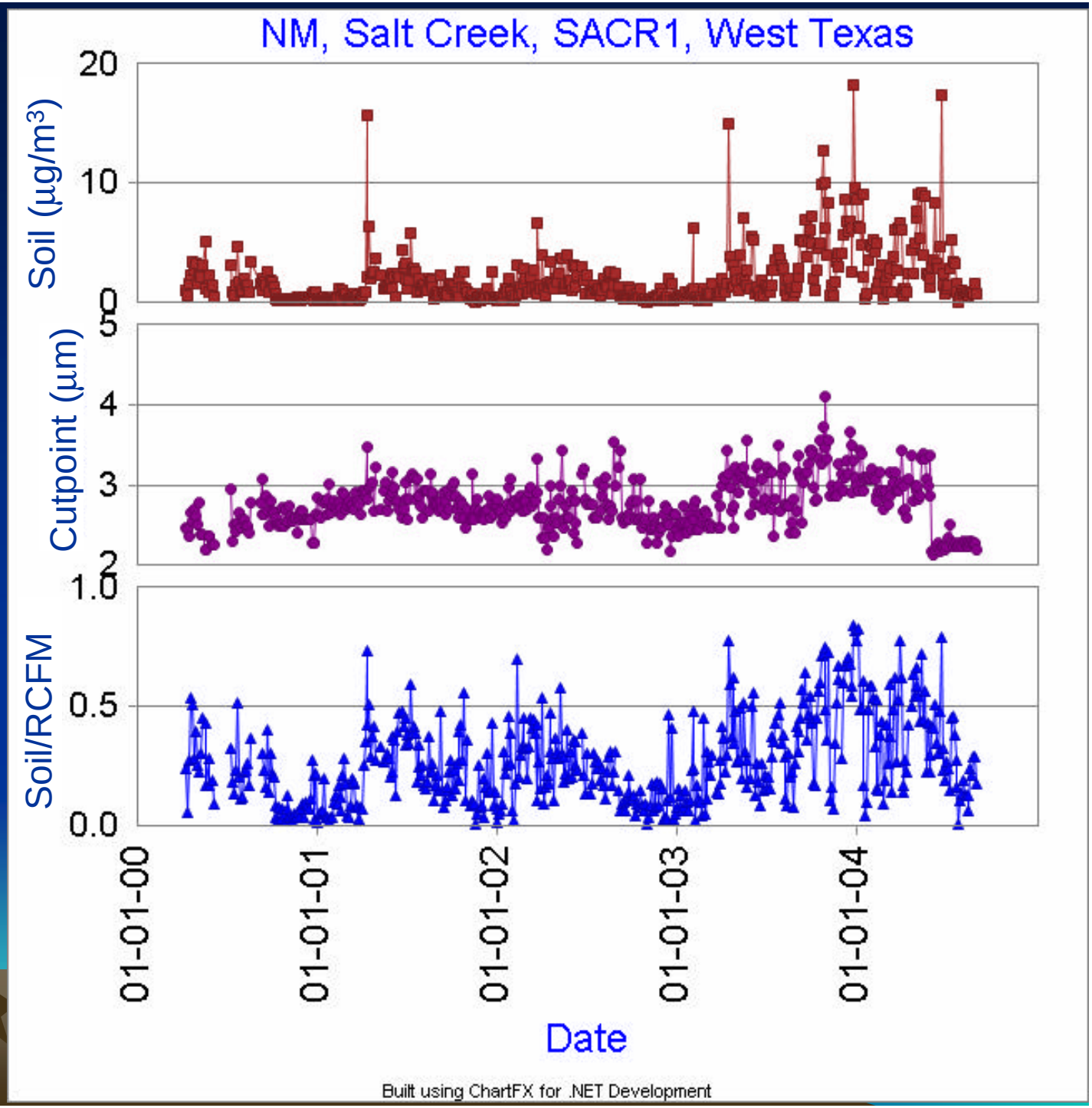


Cutpoint Variations

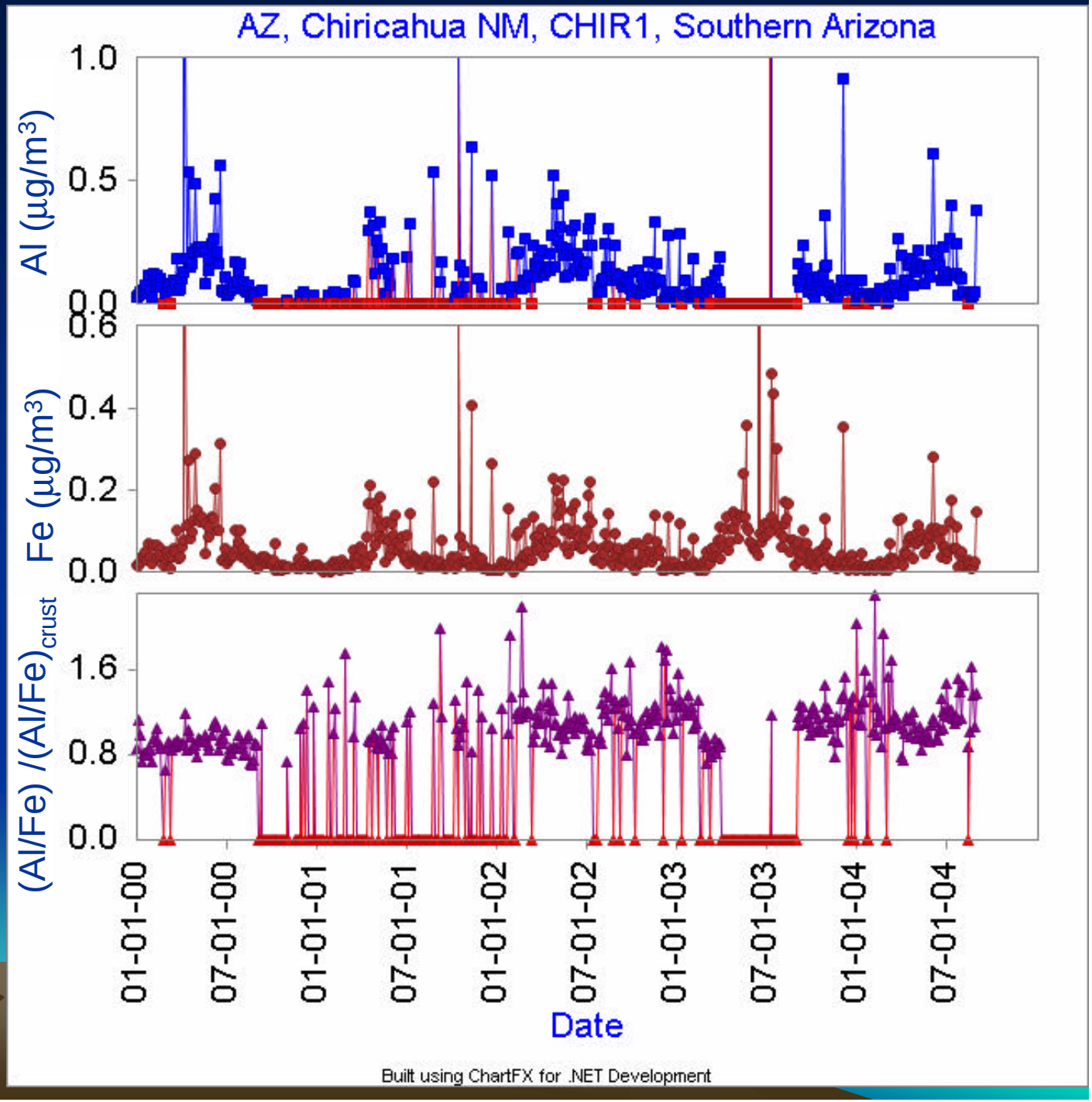




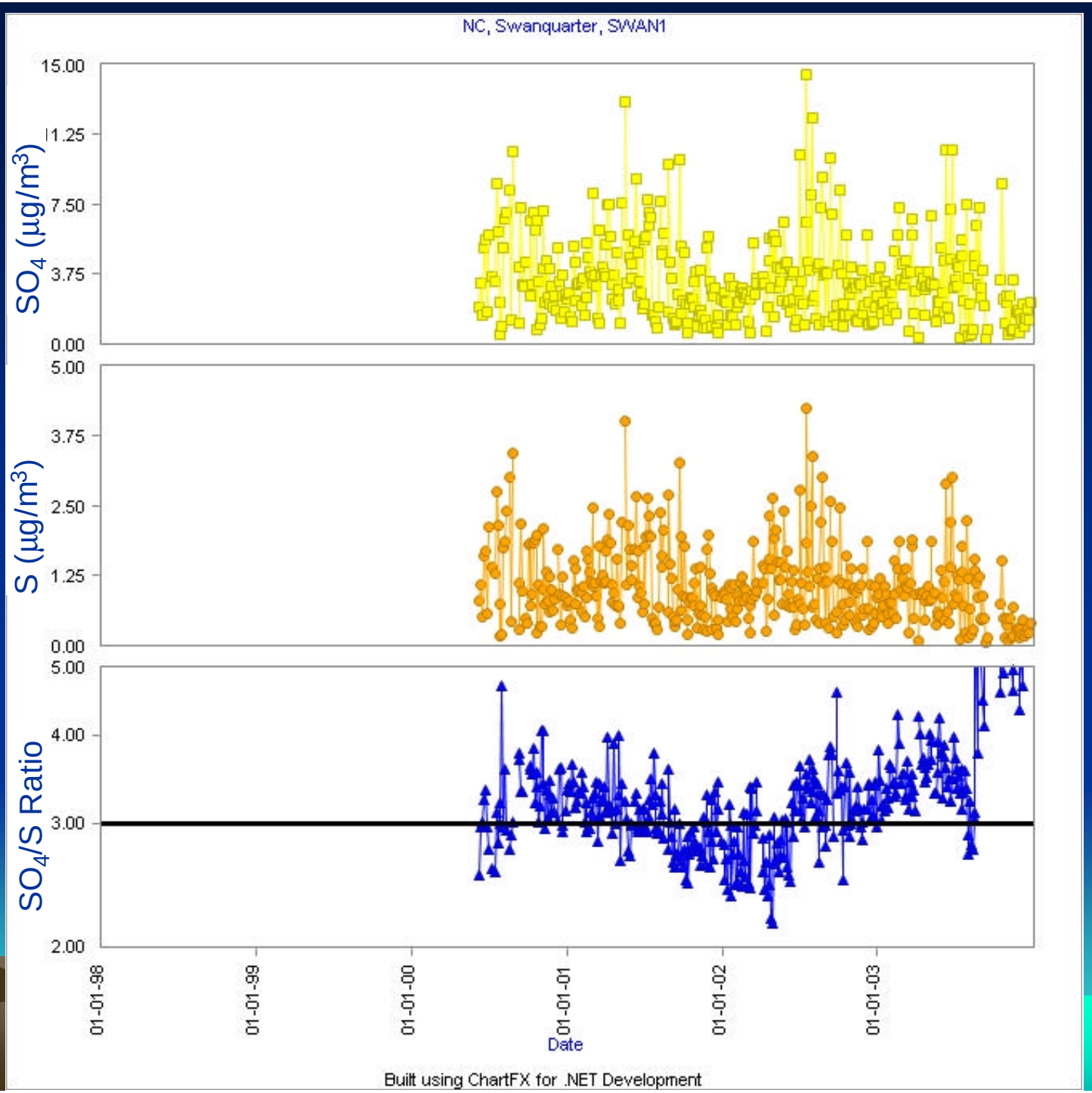
Cutpoint Variations Can Cause Misleading Trends in Soil



Aluminum Detection Problems with both PIXE and Cu XRF



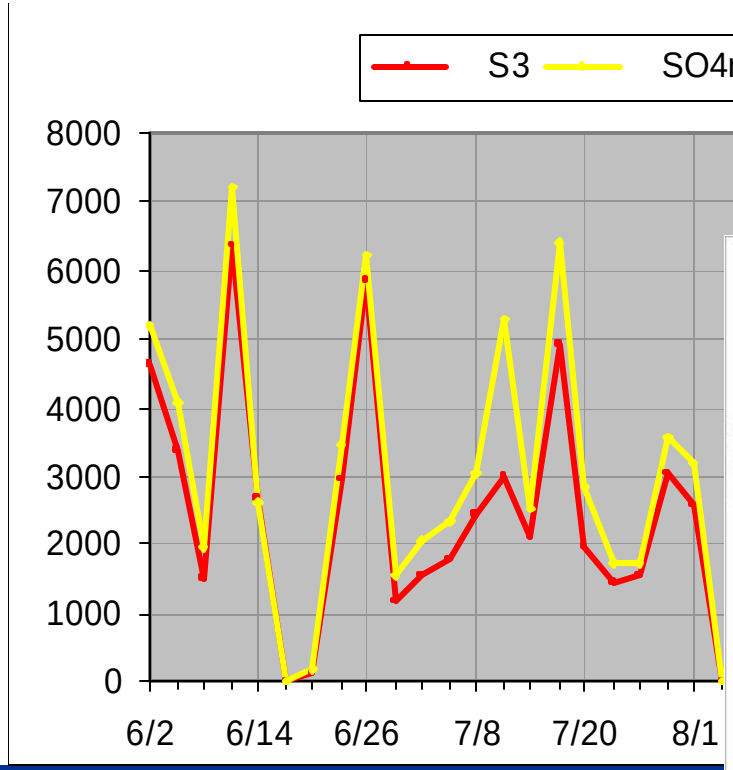
SWAN data have been removed from CIRA database



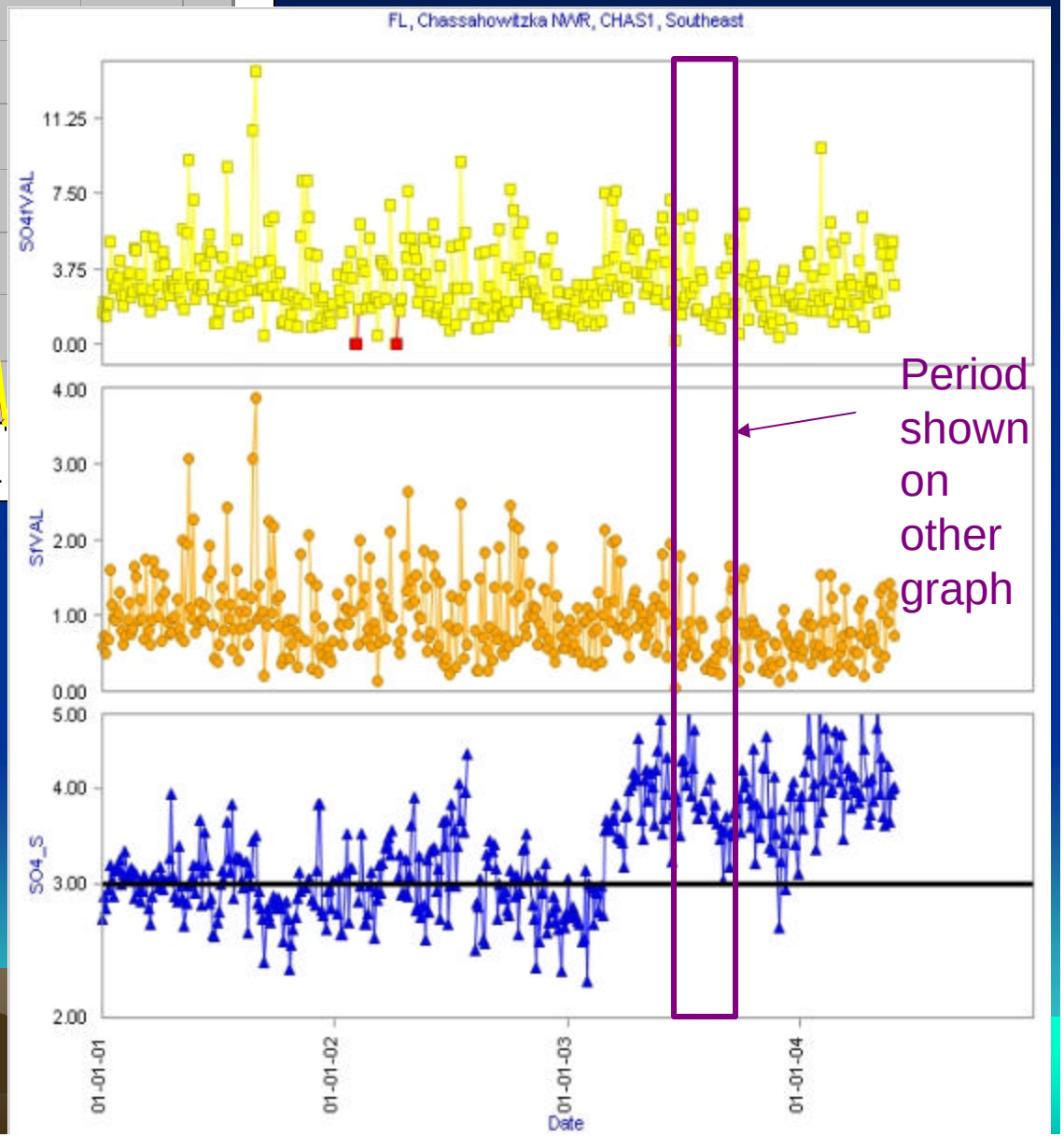
UCD Data Validation
Required Additions

- Establish objective data quality standards
  - Promote consistency over time
  - Criteria to evaluate each piece of data and data aggregation
  - Shift validation efforts to source data (e.g., flows, raw lab data, QC data)
  - Meet data delivery schedule
- Inspect data on longer time scales
- NARSTO flagging scheme

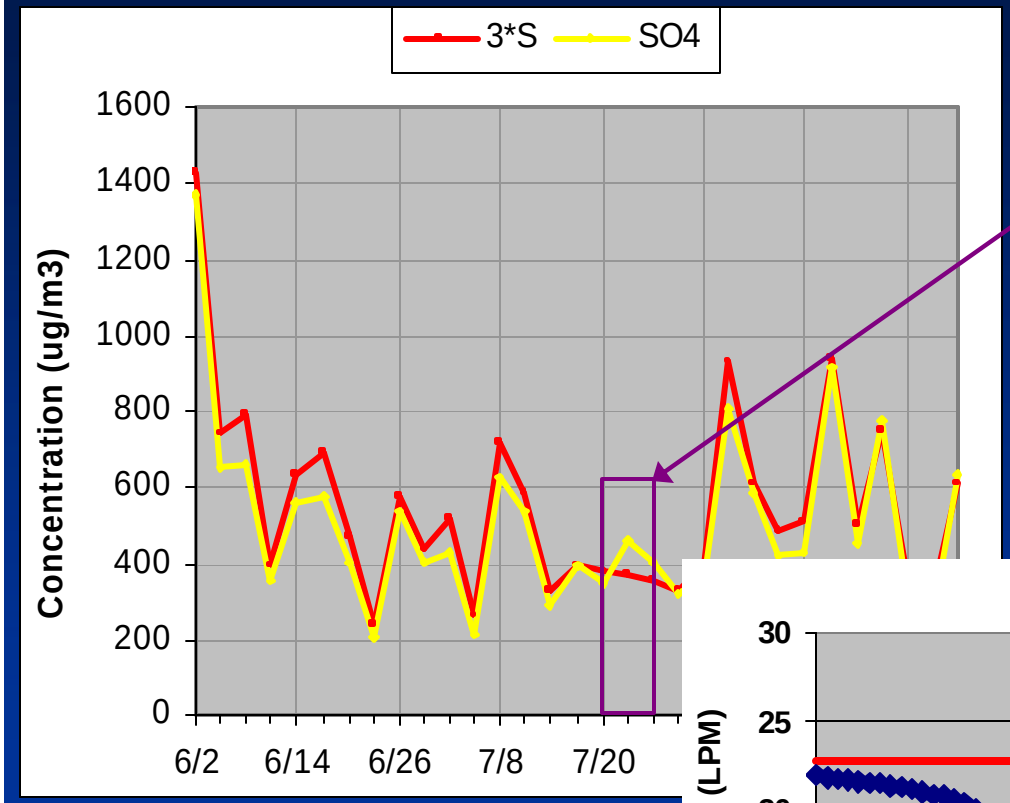
Do these data look valid?



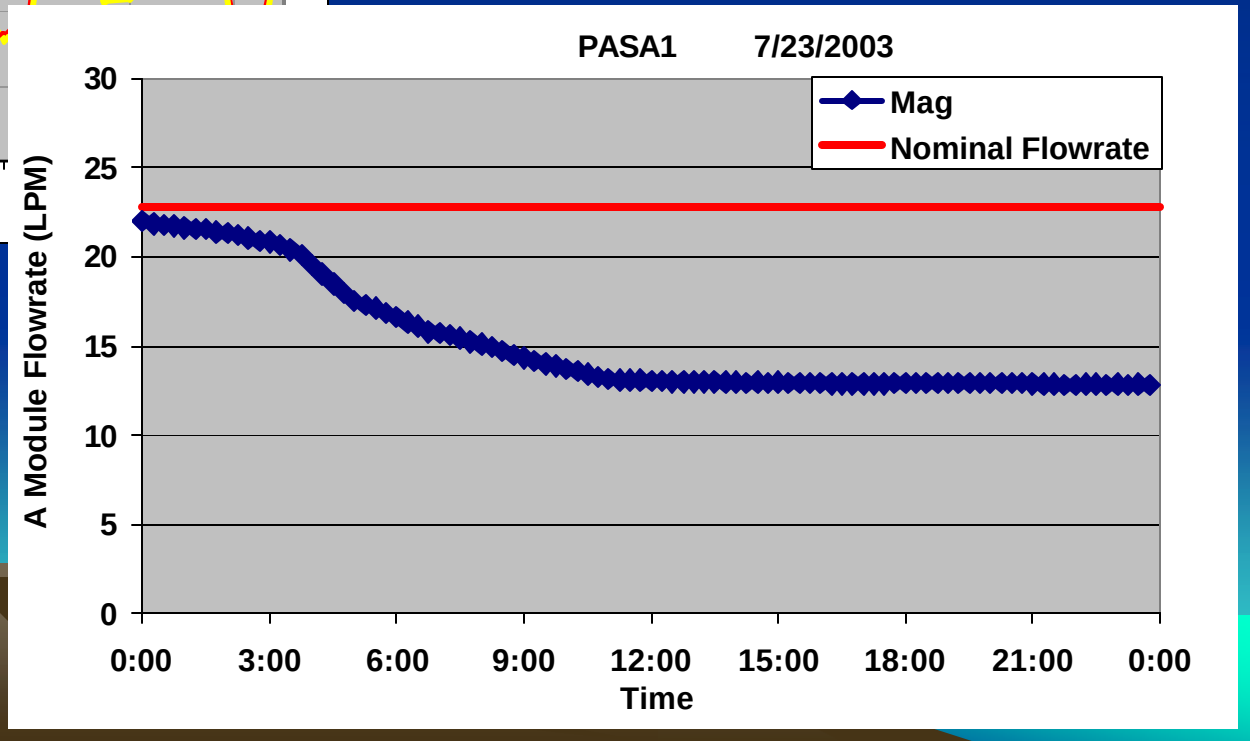
3*S and SO4 concentrations at CHAS1 from June thru August 2003



Objective Flowrate Criteria



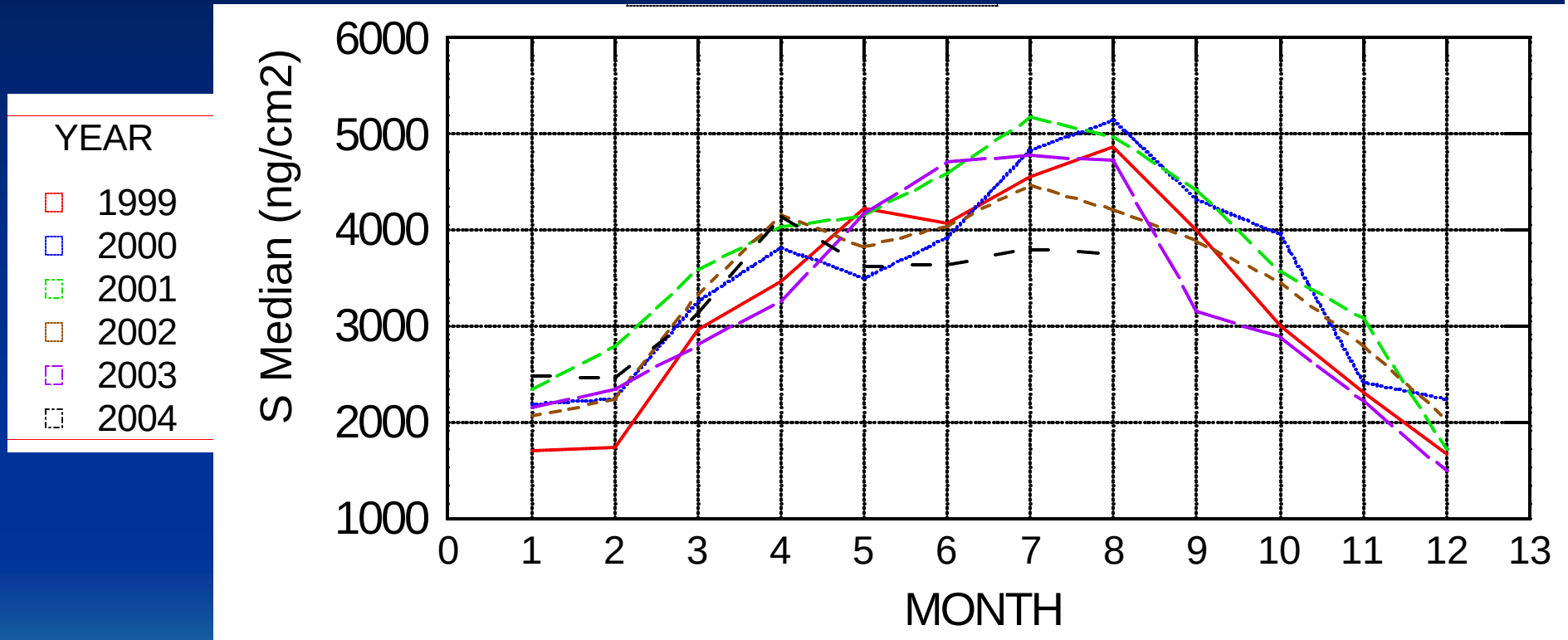
Does the 7/23/03 sulfur data look valid?



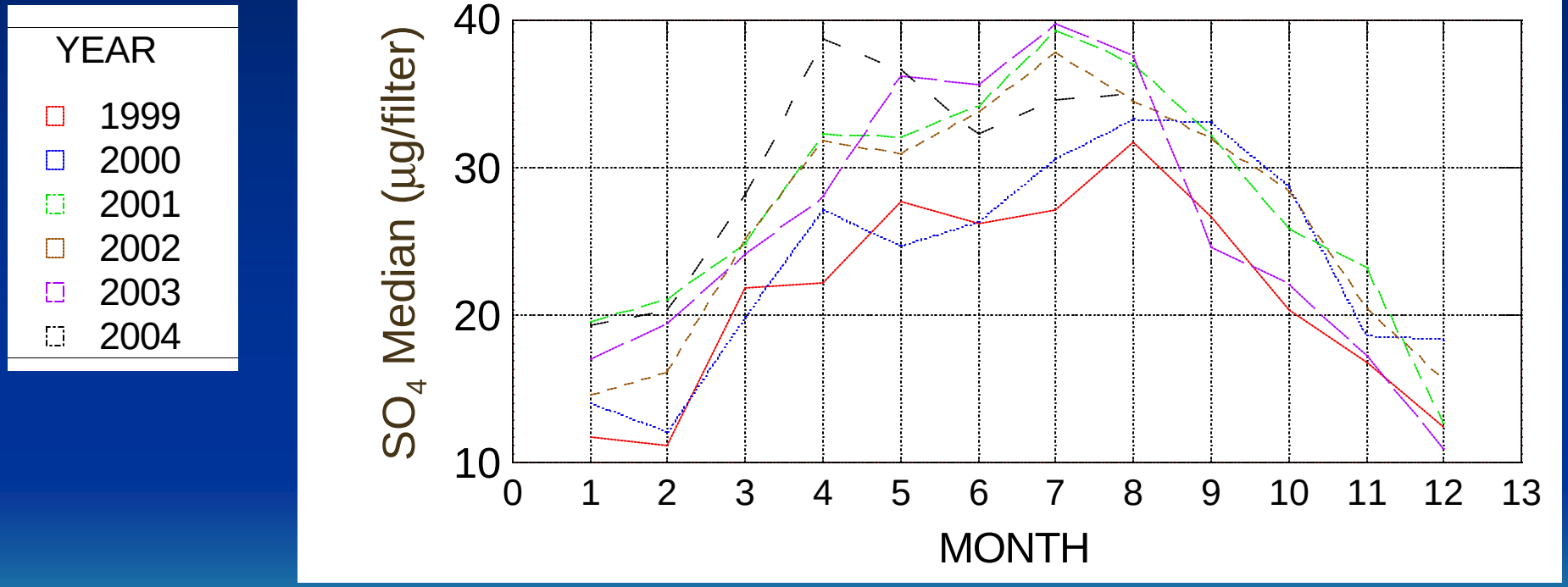
Objective Data Quality Standards

- Chemical analysis-level range checks
  - Starting with May 2004 data, the network-wide percentiles for every parameter are compared to limits based on historic values
- Site-specific range checks
  - Flowrate
    - Objective criteria established to validate the flowrate data for each individual sample
    - Need criteria to instigate action to correct chronic flow problems
  - Parameter-specific checks will be developed after the new data management system is established.

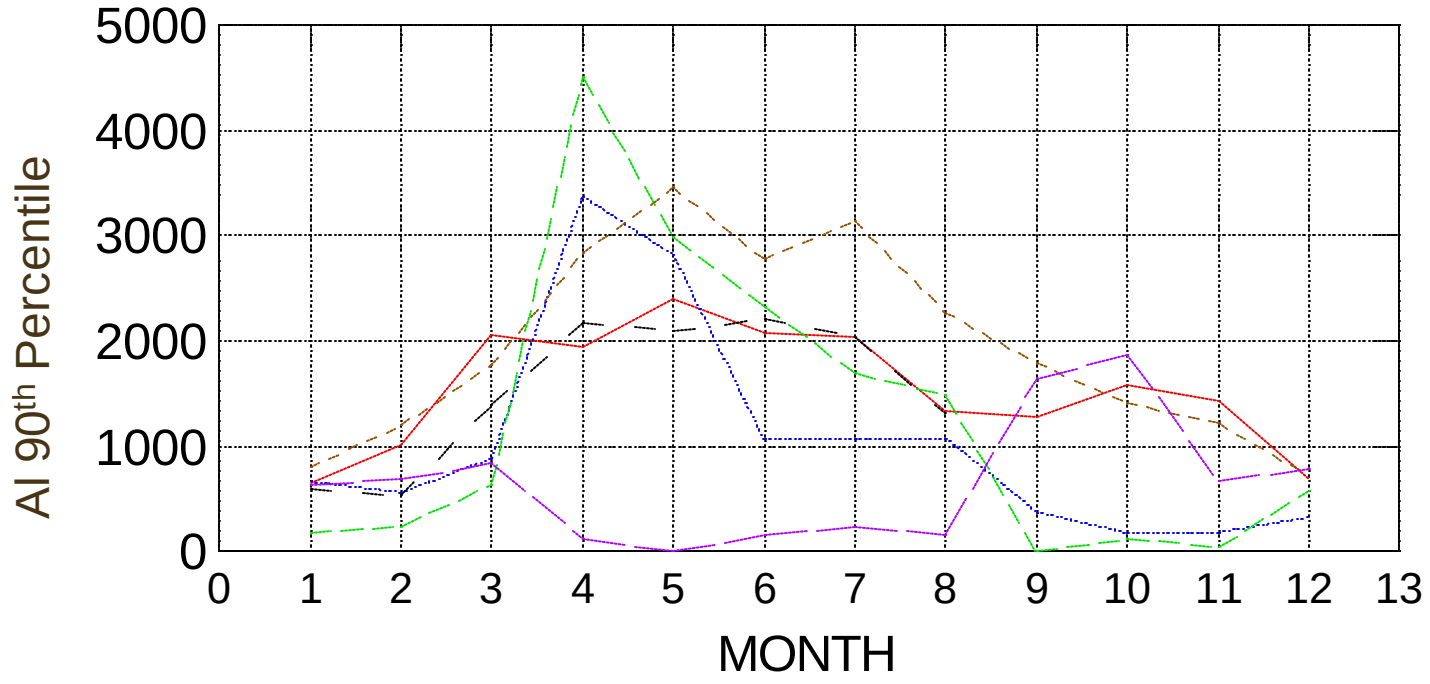
S Network-Wide Median Filter Loadings

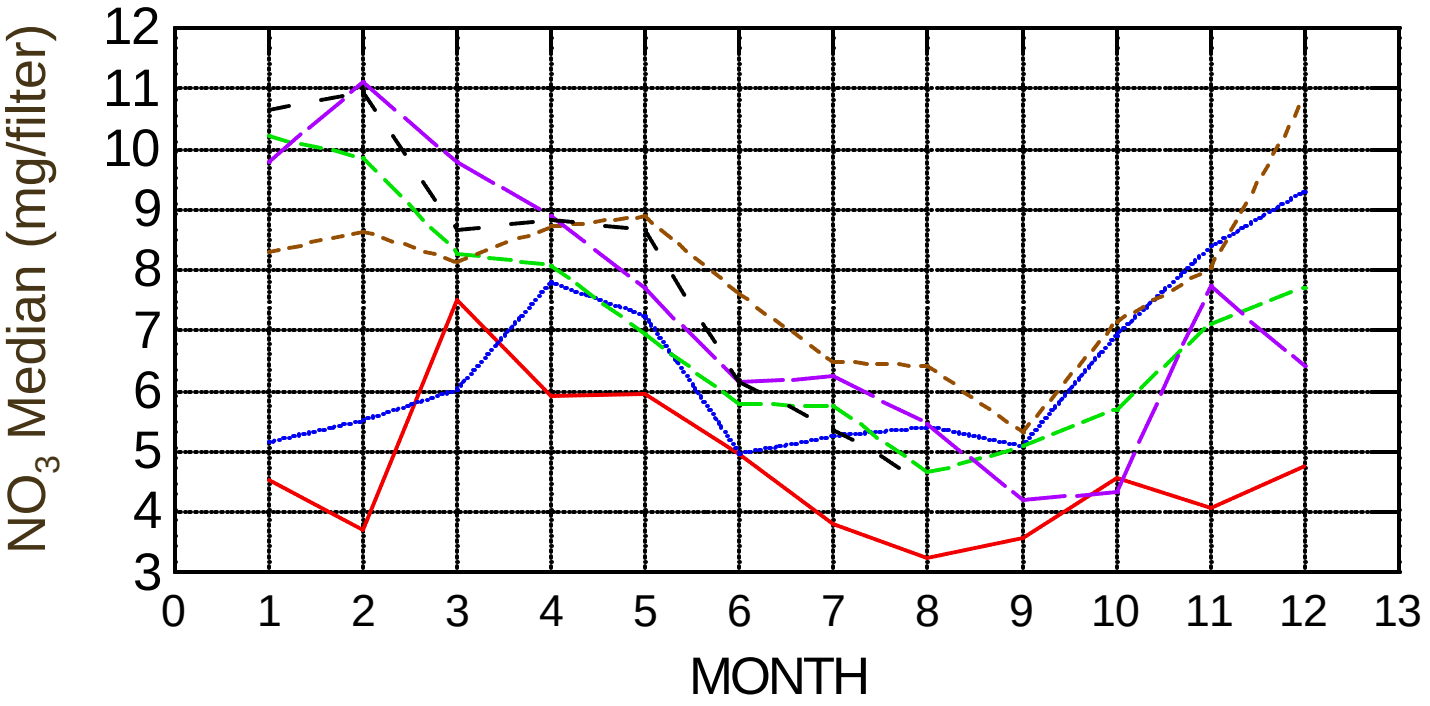


SO_4 Network-Wide Median Filter Loadings



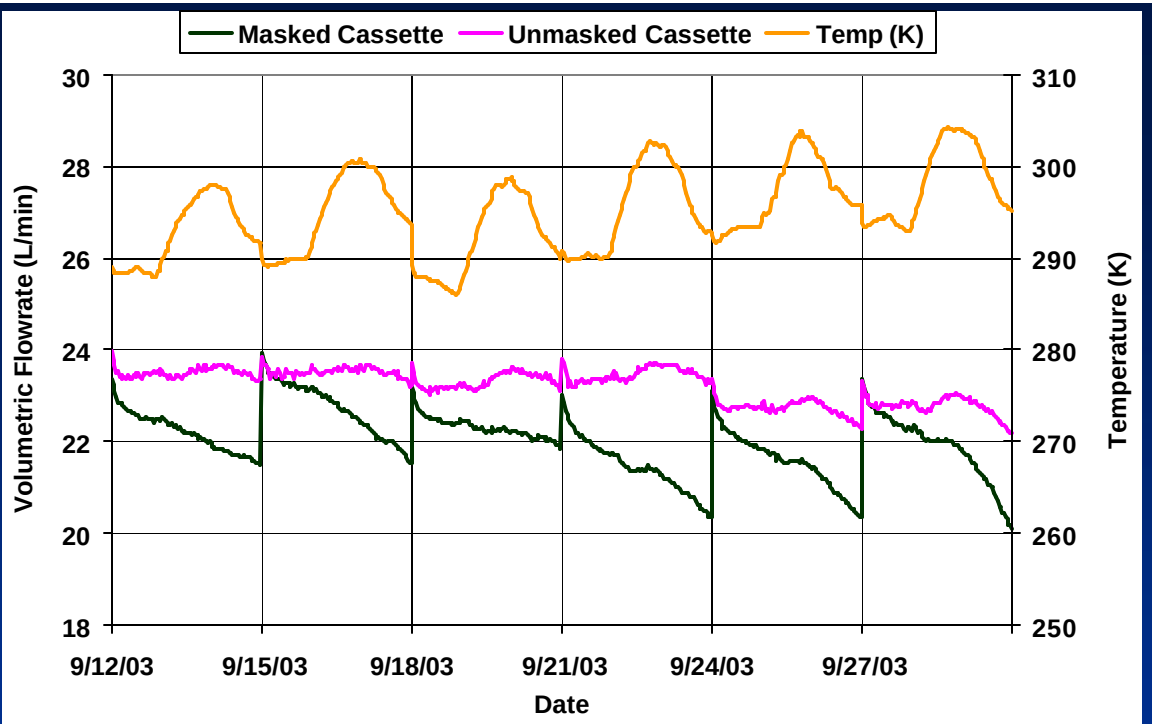
Al and NO_3 Network-Wide Filter Loadings

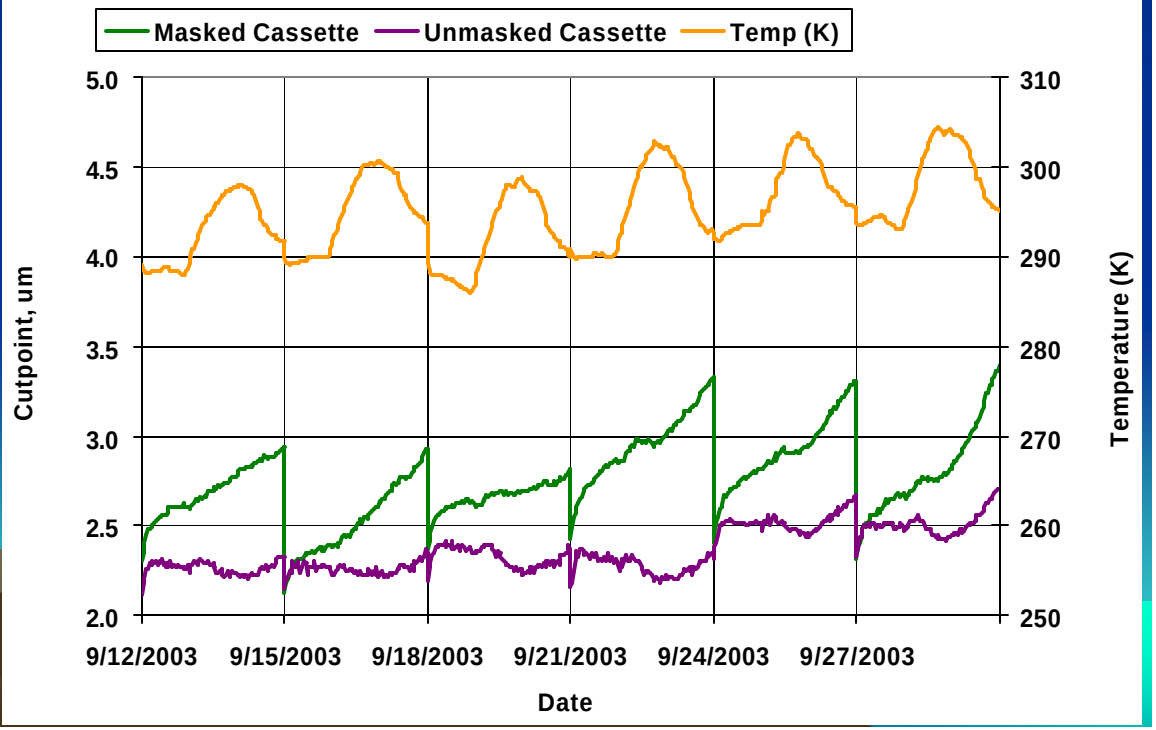




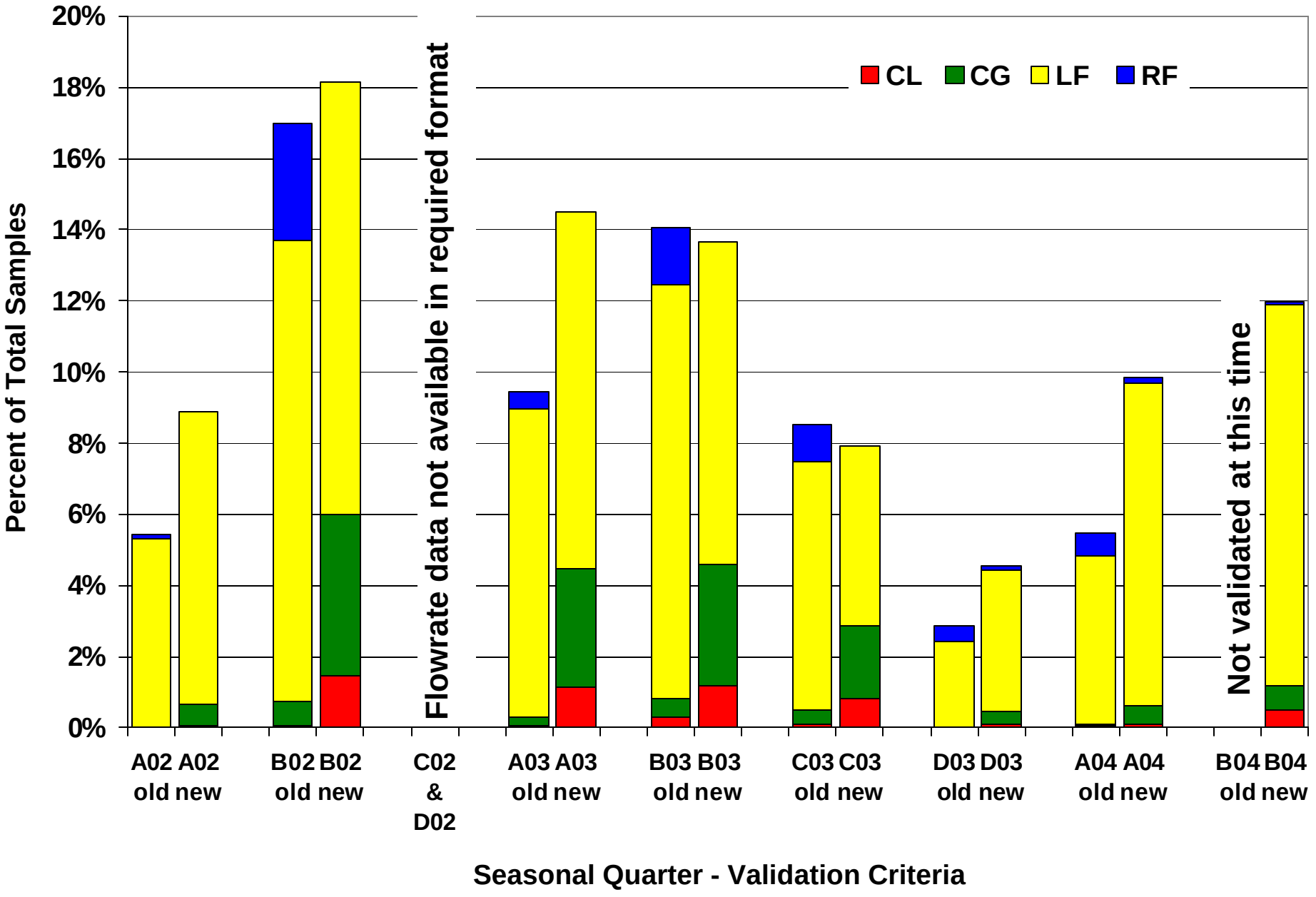
YEAR
- 1999
- 2000
- 2001
- 2002
- 2003
- 2004

Flowrate Variability with Passive Flow Control





Flowrate Validation Criteria



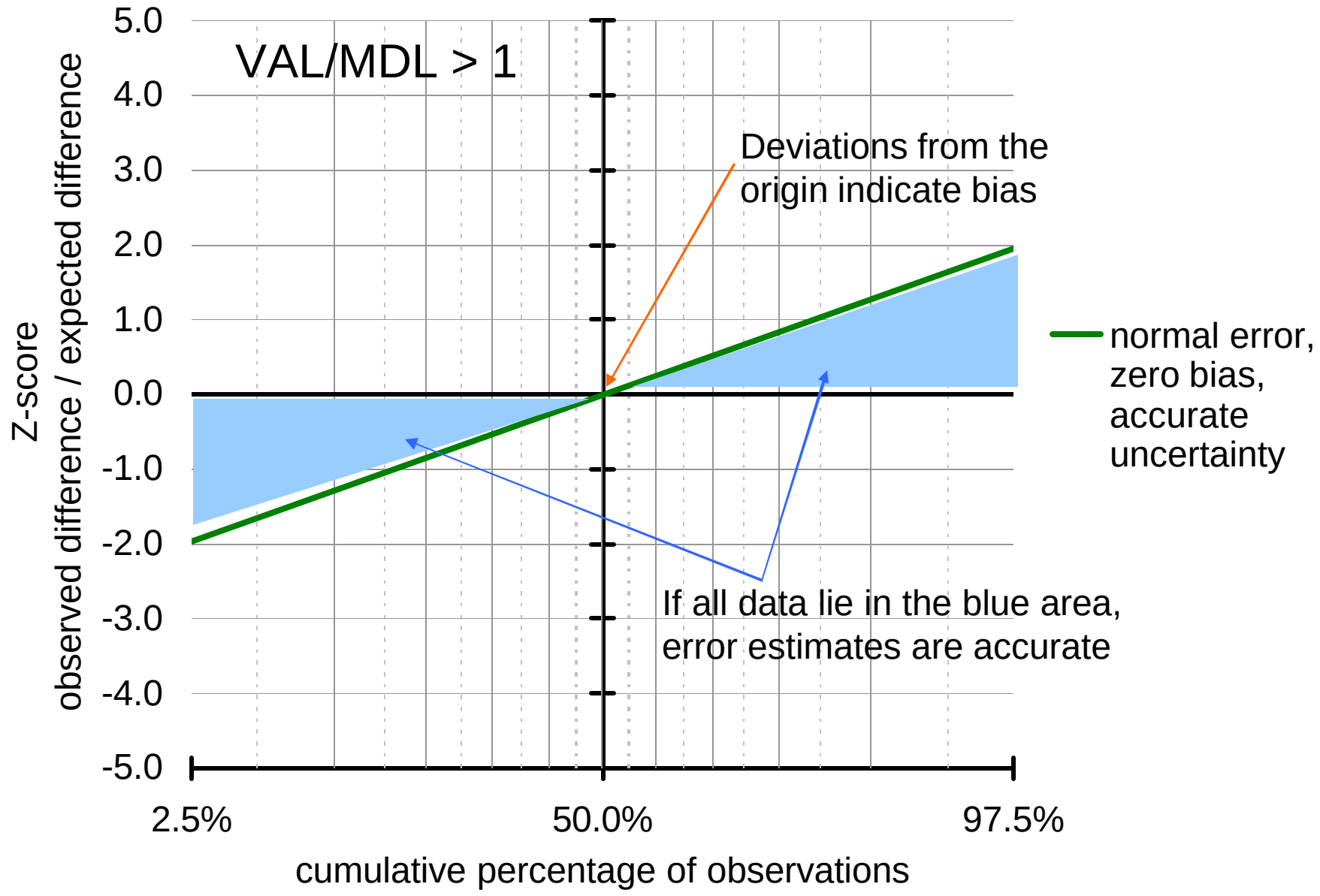
Plans for Coming Year

- I will spend majority of time on data management system design and quality control criteria development.
- Linsey will work on IMPROVE report and continue to perform secondary data validation.

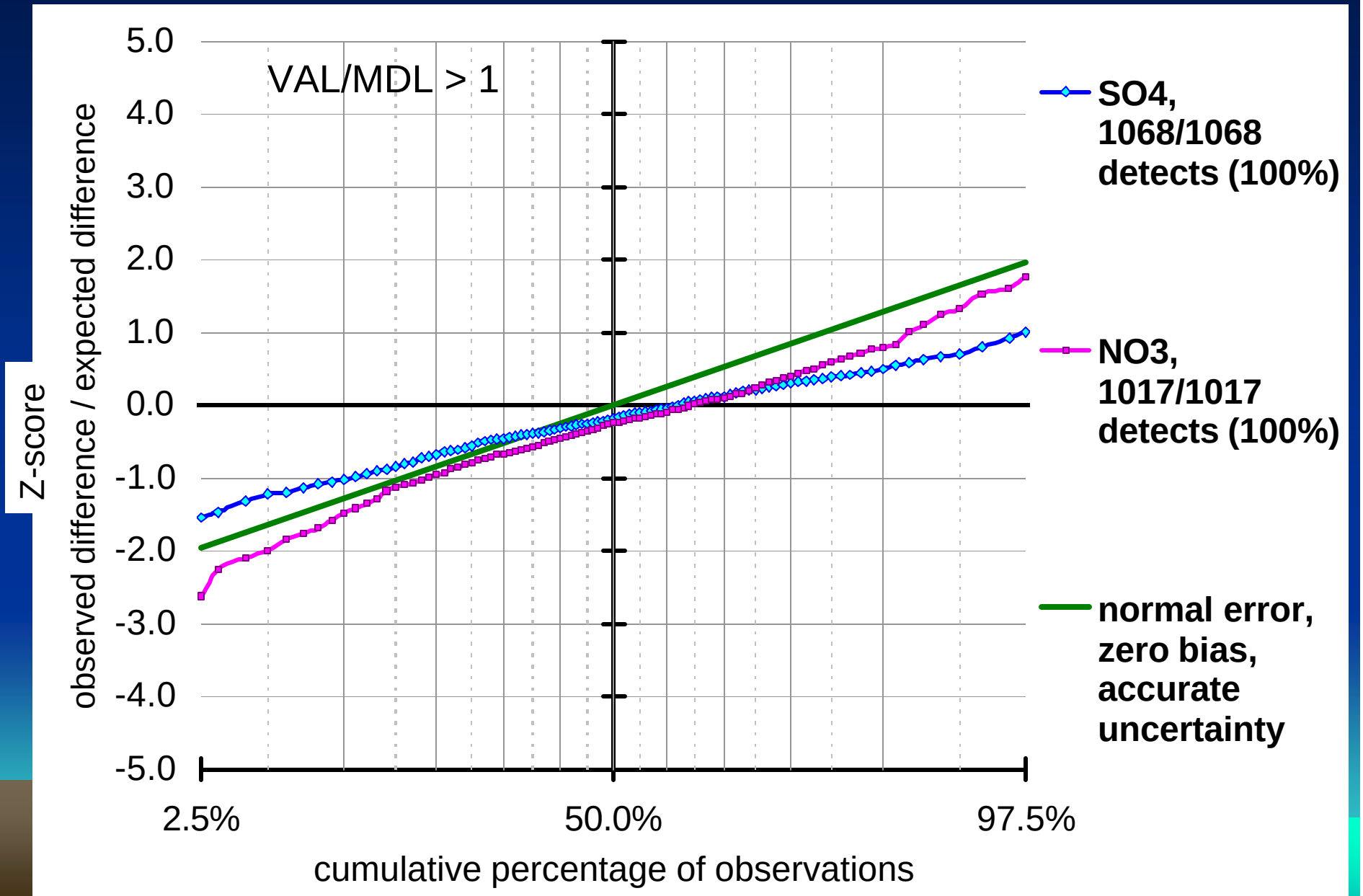
Collocated (X-module) Data

- Operating 24 collocated modules in IMPROVE network
  - Routine module is referred to as “1” module and collocated module is referred to as “x” module (e.g., MEVE1 and MEVEX)
- Collocated data have highlighted unexpected issues in the network
  - Flow differences (and concentration differences) resulting from different filter cassettes
  - Incorrectly swapped filters
  - Filters accidentally unmasked instead of masked

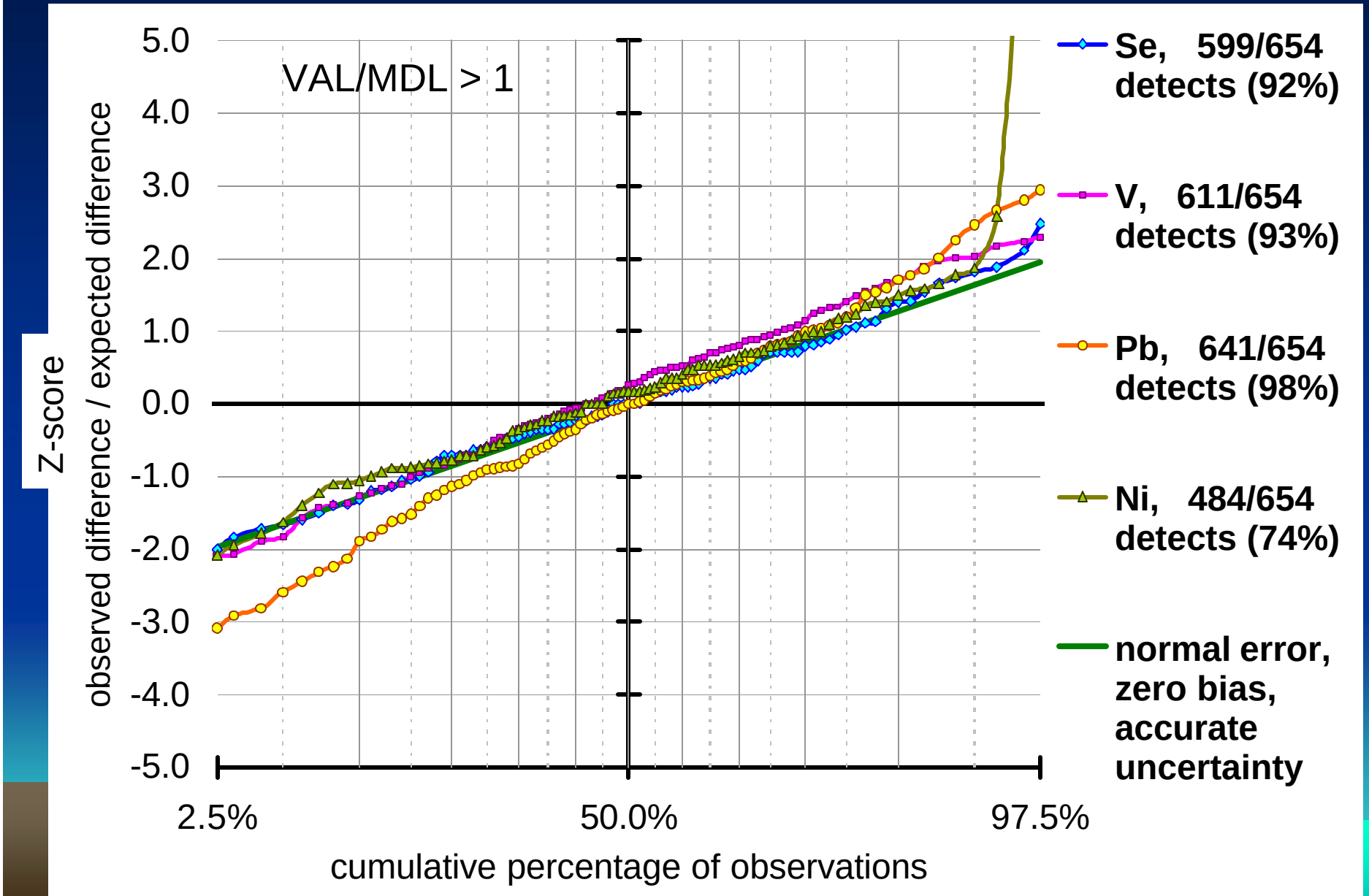
Graph Introduction



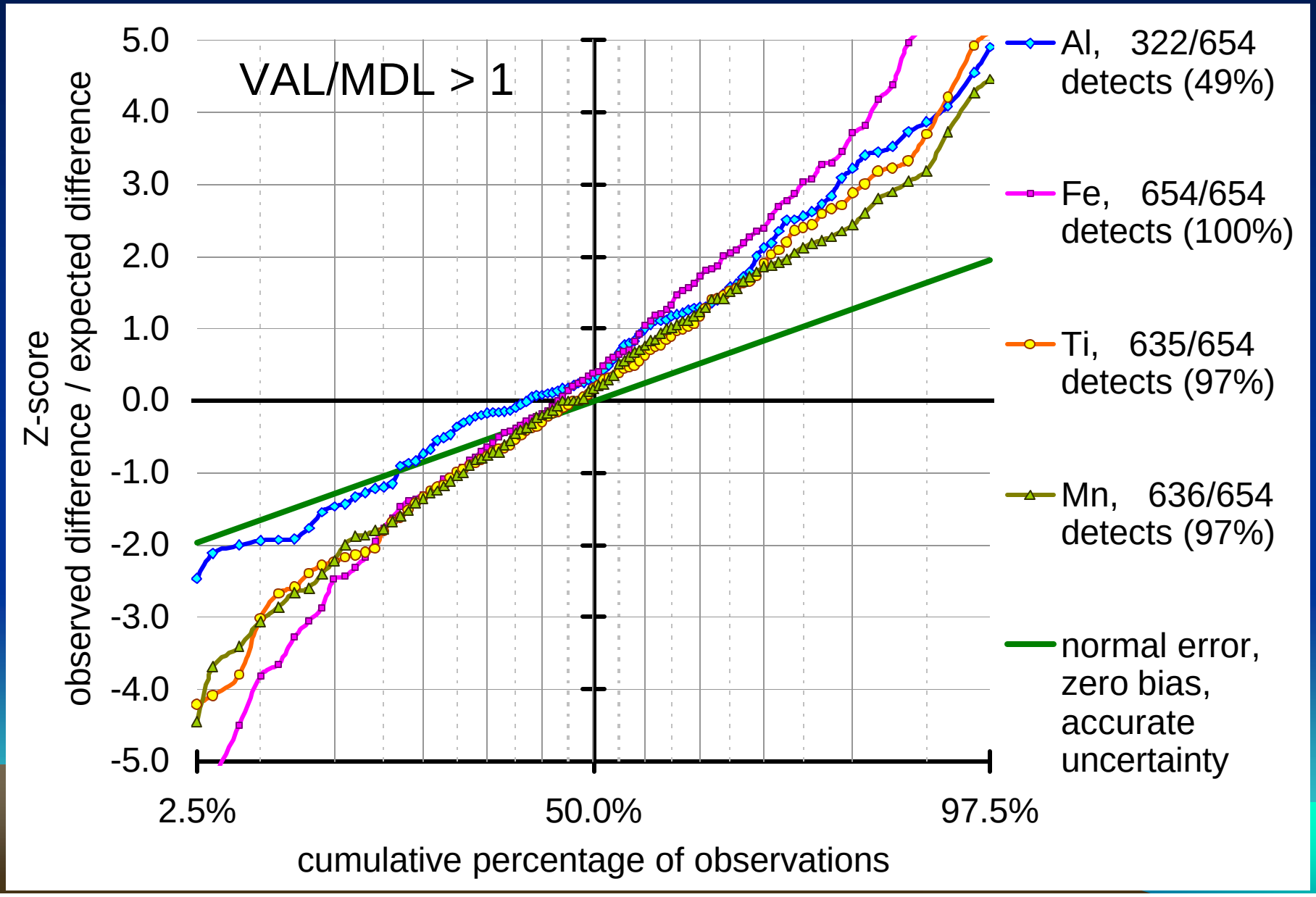
Collocated B Module Comparisons



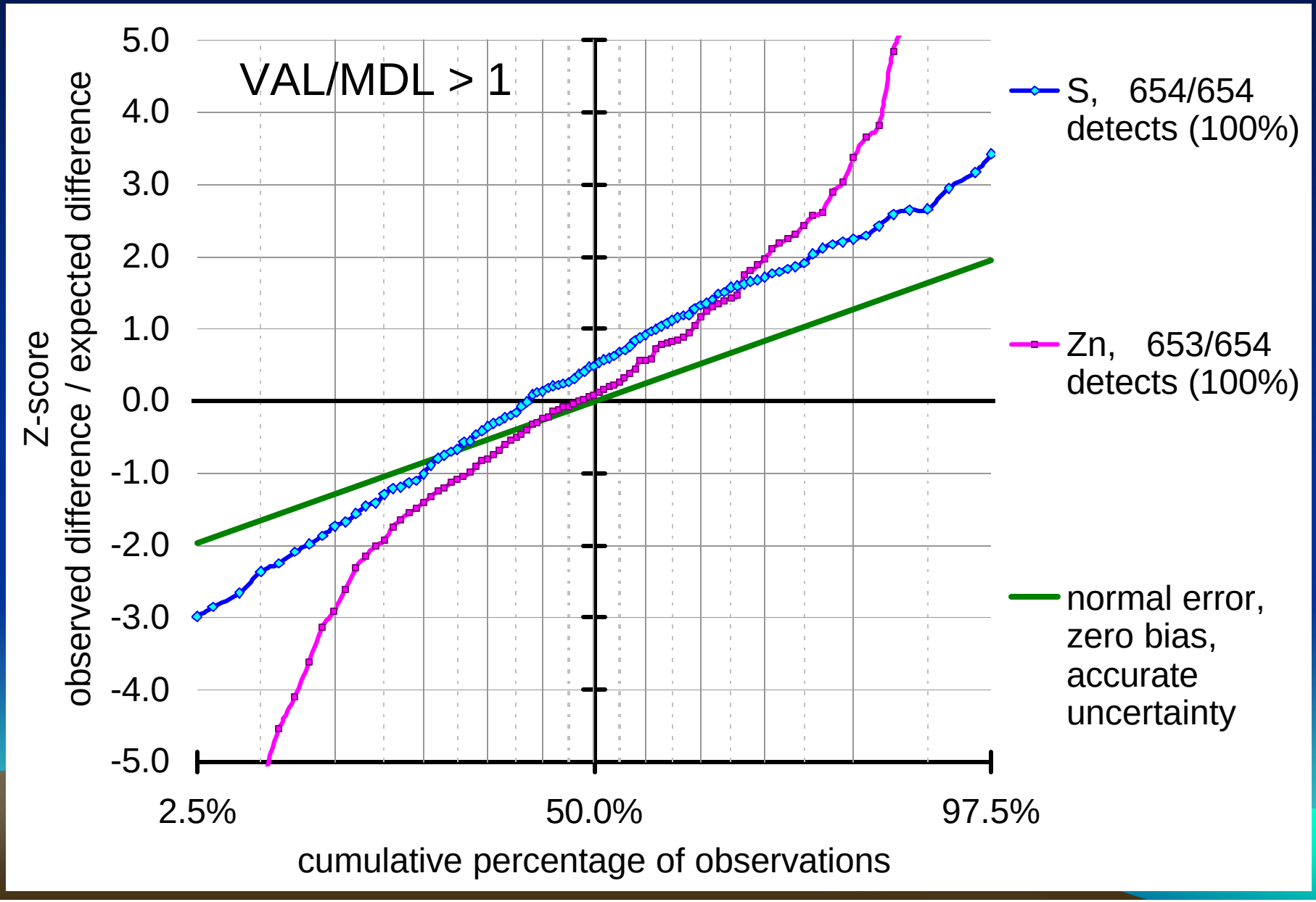
Collocated A Module Comparisons



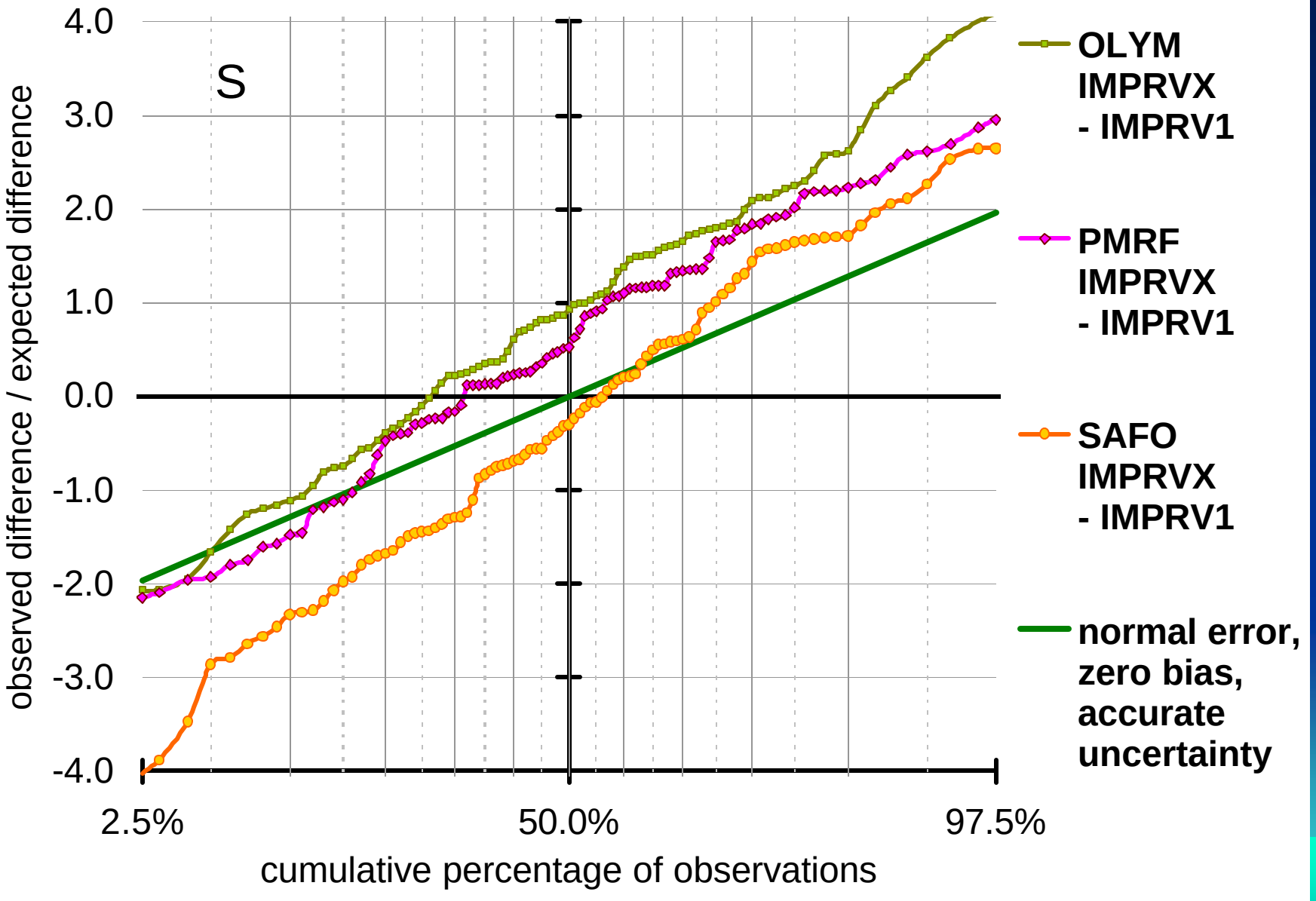
Collocated A Module Comparisons
Soil Elements



Collocated A Module Comparisons



Site-Specific A Module Comparisons



Collocated Data

- Evaluating error estimates
  - May need to consider cut-point related error for soil elements
  - Sulfur disagreement is a mystery