

Status of DUET for Tidal Data AMQAW 11 July, 2013 Mary Ellen Ley, Mike Mallonee

### Scope of Project

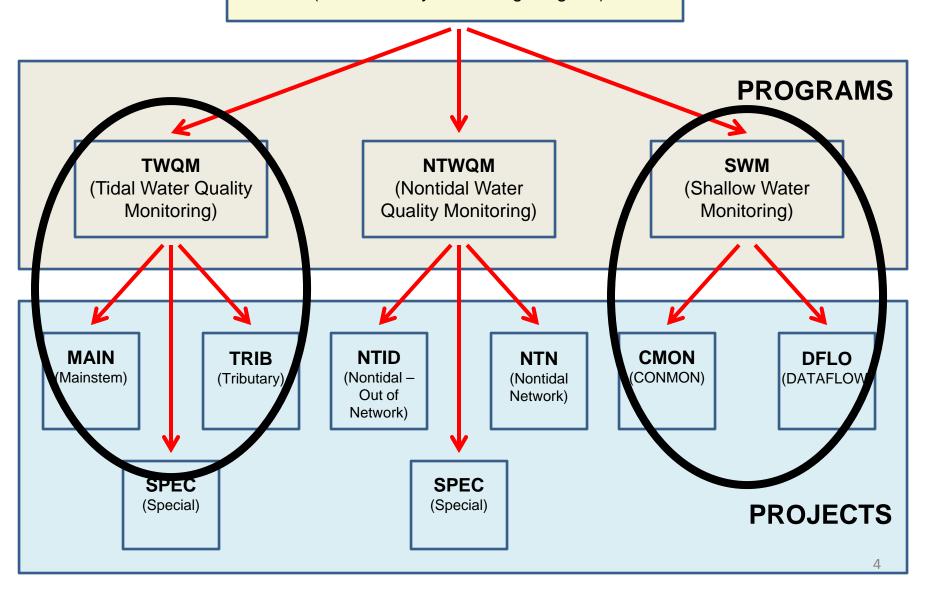
- DUQAT (Data Upload and Quality Assurance Tool) is currently used to upload tidal data submittals for Maryland and Virginia to the CBP Water Quality Database.
- Project will develop DUET (Data Upload and Evaluation Tool)
  - Revise DUQAT to enable the submission, review, transformation, and archival of WQ data and the metadata for the Tidal Water Quality Monitoring (TWQM) and Shallow Water Monitoring (SWM) Programs.
  - DUET will upload TWQM and SWM data and metadata from the 4 Agencies (Data Providers) collected by 6 Sources (Data Collectors).

## Scope of Project (2)

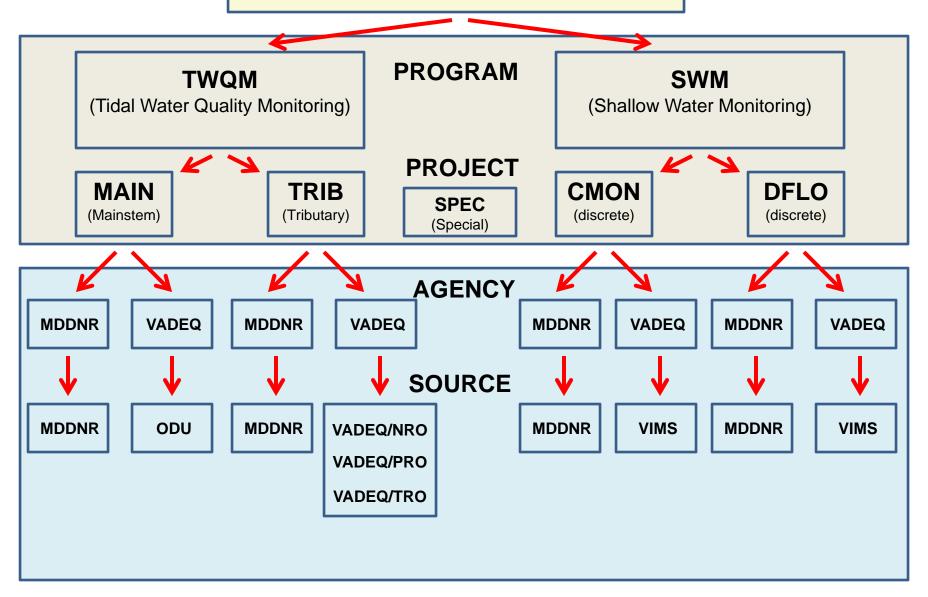
- Submitted WQ data will be reviewed by DUET, and generate reports with metadata on the following:
  - Timeliness of the Source Submissions and the Agency Uploads.
  - Completeness of the submitted data, in relation to the data expected.
  - Quality of the submitted data (e.g. clerical errors, extreme values, logic checks (dissolved < whole), and data accuracy (bias and precision)).
- QC'd data and metadata will be archived in CIMS.
  - Goal is to process the data with DUET beginning with October 2013 data submittals.

# WQ\_1 CBP Water Quality Database

(Water Quality Monitoring Program)



# WQ\_1 CBP Water Quality Database (Tidal Data)



#### Tidal DUET Parameter Completeness

TIDAL METADATA				FIELD PARAMETERS (ISM)								
PROGRAM	PROJECT	AGENCY	SOURCE	WTEMP	SPCOND		DO	PH	SALINITY	SECCHI	PN	TDN
			Т	WATER EMPERATURE	CONDUCTIVITY	O	SOLVED XYGEN ENTRATION	рН	SALINITY	SECCHI	PARTICULATE NITROGEN	TOTAL DISSOLVED NITROGEN
TWQM	MAIN	MDDNR	MDDNR	X	X		X	X	X	X	X	X
TWQM	TRIB	MDDNR	MDDNR	X	X		X	X	X	X	X	X
SWM	CMON	MDDNR	MDDNR	X	X		X	X	X	X	X	X
SWM	DFLO	MDDNR	MDDNR	X	X		X	X	X	X	X	X
TWQM	MAIN	VADEQ	ODU	X	X		X	X	X	X	X	X
TWQM	TRIB	VADEQ	VADEQ/***	X	X		X	X	X	X	X	X
SWM	CMON	VADEQ	VIMS	X		X		X	X	X		
SWM	DFLO	VADEQ	VIMS	X	X		X	X	X	X		
NH4F	NO2F	NO23F	PP	TDP	PO4F		TSS	FSS	VSS	PC	CHLA	PHEO
AMMONIUM NITROGEN AS N (FILTERED)	NITRITE NITROGEN AS N (FILTERED)	NITRATE PLUS NITRITE NITROGEN AS N (FILTERED)	PARTICULATE PHOSPHORUS	TOTAL DISSOLVED PHOSPHORUS	ORTHOPHOSI PHOSPHORU (FILTERE	S AS P	TOTAL SUSPENDED SOLIDS	FIXED SUSPENDE SOLIDS	VOLATILE SUSPENDED SOLIDS	PARTICULATE CARBON	CHLOROPHYLL A	PHEOPHYTIN
X	X	X	X	X	X		X		X	X	X	X
X	X	X	X	X	X		X		X	X	X	X
X	X	X	X	X	X		X		X	X	X	X
X	X	X	X	X	X		X		X	X	X	X
X	X	X	X	X	X		X	X		X	X	X
X	X	X	X	X	X		X	X		X	X	X
							X	X	X		X	X
							X	X	X		X	X

#### **DUET Calculated Parameters**

Calculated Value	Expected Calculation	MARYLAND (MDDNR)				VIRGINIA (ODU, VADEQ*, VIMS, VIMS)			
		MAIN	TRIB	CMON	DFLO	ODU	TRIB	CMON	DFLO
DIN	DIN = NH4F + NO23F	yes	yes	yes	yes	yes	yes		
DON	DON = TDN - NH4F - NO23F	yes	yes	yes	yes	yes	yes		
DOP	DOP = TDP - PO4F	yes	yes	yes	yes	yes	yes		
FSS	FSS = TSS - VSS								
KD		yes		yes	yes	yes	yes	yes	
NO3F	NO3F = NO23F - NO2F	yes	yes	yes	yes	yes	yes		
SIGMA-T		yes	yes	yes	yes	yes	yes	yes	yes
TN	TN = PN + TDN	yes	yes	yes	yes	yes	yes		
TON	TON = PN + TDN - NH4F - NO23F	yes	yes	yes	yes	yes	yes		
TP	TP = PP + TDP	yes	yes	yes	yes	yes	yes		
VSS	VSS = TSS - FSS								

#### Consistency Checks: Problem codes

PROBLEM	DESCRIPTION
	CONSISTENCY CHECK PROBLEM CODES
QQ	PART EXCEEDS WHOLE VALUE YET DIFFERENCE IS WITHIN ANALYTICAL PRECISION (PQL OR REPORTING LIMIT)
NQ	PART EXCEEDS WHOLE VALUE AND DIFFERENCE IS NOT WITHIN ANALYTICAL PRECISION
IQ	CANNOT DETERMINE IF PART EXCEEDS WHOLE VALUE AND WHETHER OR NOT DIFFERENCE IS WITHIN ANALYTICAL PRECISION
NV	NEGATIVE CALCULATED VALUE IS VALID GIVEN PRECISION OF MEASURED WATER QUALITY PARAMETERS; ACTUAL CALCULATED CONCENTRATION LIKELY IS LOW; POSSIBLY LESS THAN PQLS OF MEASURED WATER QUALITY PARAMETERS

EXCEPTION: Report all "NQ" Duplicate Sample data (regardless of consistency check results).

#### Consistency Check Example

"I have a PO<sub>4</sub> result of 0.024 mg/L, which is higher than the TDP result of 0.014. Is this a case where I would delete both values, based on what has been proposed under the ESAR DUET?"

 $PO_4$  RL = 0.004 mg/L TDP RL = 0.010 mg/L

Use the higher RL to assess difference; Here difference must be < 0.010 mg/L

$$[PO4] - [TDP] = 0.024 - 0.014 = 0.010 \text{ mg/L}$$

The difference is exactly the same as the TDP reporting limit. However, the criterion for QQ is < RL, not  $\le$  RL. Therefore, without additional information from the lab, you would withhold the data and assign a "NQ" problem code.

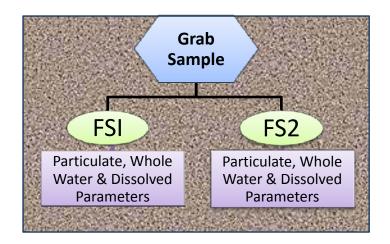
Alternatively, you could have the lab investigate the inconsistency in results and see if there was a reporting error, or if there is a reason to justify keeping data, e.g., Reporting limits may have changed, one test may have been off, etc.

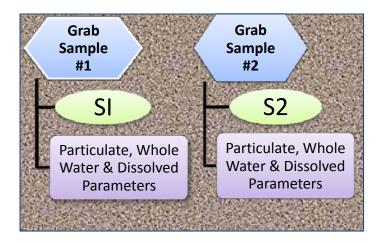
#### **DUET Qualifier Codes**

QUALIFIER_ID	QUALIFIER	DESCRIPTION
1	<	Concentration is less than method detection limit
2	>	Concentration not quantified; exceeds given value (eg.FCOLI).
3	G	REPORTED VALUE IS BETWEEN THE MDL AND THE PRACTICAL QUANTITATION LEVEL (OR REPORTING LIMIT)

#### Field Replicate Samples

- 1.Field Split (FS1 & FS2): Two representative portions are taken from one homogeneous sample and processed identically.
- 2.Field Duplicate, Co-located (S1 & S2): A sample taken at the same sample location and depth as a CBP sample. The sample and duplicate shall be taken in quick succession of each other.
- 3. The minimum frequency for collecting Field Split or Field Duplicate samples is according to the CBP monitoring program:
  - a. Mainstem Monitoring: Collect a field split or a field duplicate once for every 20 samples.
  - b. Tidal Tributary Monitoring: Collect field splits once per month, from both surface and bottom depths.





#### Field Blanks

#### Field Blanks

- 1. The frequency for preparing field-filtered blanks is according to the CBP monitoring program:
  - a. Mainstem Monitoring: Prepare one field-filtered blank each day.
  - b. Tidal Tributary Monitoring: Prepare at least one field-filtered blank per month
- 2. If the concentration of a field blank exceeds the MDL (?), reporting level or the lowest analytical standard in the calibration curve, field and/or laboratory contamination should be suspected and corrective action initiated.
- 3. Corrective action includes an investigation of possible contamination sources (e.g., instrument calibration check, field blank water, sample containers, etc.) and procedural modifications if necessary.

#### Tidal DUET Problem Codes

PROBLEM	DESCRIPTION
Α	LABORATORY ACCIDENT
AA	FIELD ACCIDENT
В	CHEMICAL MATRIX INTERFERENCE
	SPURIOUS OR PERSISTENT CONTAMINATION THAT APPEARS TO AFFECT BLANKS ONLY. CONTAMINATION IS RELATED TO THE MANNER OR EQUIPMENT
BB	OR SUPPLIES USED TO OBTAIN THE BLANK; SUCH AS CONTAMINATED SOURCE WATER
	BIASED MEASUREMENT; CONCENTRATION COULD REFLECT CONTAMINATION BIAS; ASSOCIATED FIELD BLANK CONCENTRATIONS WERE WITHIN SAME
BM	MAGNITUDE AND COULD CONTRIBUTE AT LEAST 10% TO THE MEASURED WATER QUALITY PARAMETER CONCENTRATION
С	INSTRUMENT FAILURE
	SPURIOUS OR PERSISTENT CONTAMINATION; WHICH APPEARS TO REFLECT THE MANNER OR EQUIPMENT OR SUPPLIES USED TO OBTAIN BLANKS AND
CB	ASSOCIATED WATER QUALITY SAMPLES
CC	CANNOT CALCULATE GIVEN AVAILABLE DATA
D	INSUFFICIENT SAMPLE
DD	SAMPLE SIZE NOT REPORTED (ASSUMED)
E	SAMPLE RECEIVED AFTER HOLDING TIME
F	POST-CALIBRATION FAILURE LIKELY DUE TO EQUIPMENT DAMAGE AFTER SAMPLING; DATA APPEAR NORMAL
FF	MEAN REPORTED DUE TO POOR REPLICATION BETWEEN PADS
G	REPORTED VALUE IS BETWEEN MDL AND THE PRACTICAL QUANTITATION LEVEL (OR REPORTING LIMIT); 12/17/10
GG	SAMPLE ANALYZED AFTER HOLDING TIME
HI	HIGH RELATIVE PERCENT DIFFERENCE IN DUPLICATE SAMPLE MEASUREMENTS
I	SUSPECT VALUE HAS BEEN VERIFIED CORRECT
IQ	CANNOT DETERMINE IF PART EXCEEDS WHOLE VALUE AND WHETHER OR NOT DIFFERENCE IS WITHIN ANALYTICAL PRECISION
J	INCORRECT SAMPLE FRACTION FOR ANALYSIS
JJ	VOLUME FILTERED NOT RECORDED (ASSUMED)
L	LICOR CALIBRATION OFF BY >= 10% PER YEAR. USE WITH CALC KD WHERE PROB OF LU, LS, LB EXIST IN RAW
LB	LICOR CALIBRATION OFF BY >= 10% PER YEAR FOR BOTH AIR AND UPWARD FACING SENSORS
LS	LICOR CALIBRATION OFF BY >= 10% PER YEAR FOR AIR SENSOR
LU	LICOR CALIBRATION OFF BY >= 10% PER YEAR FOR UPWARD FACING SENSOR
MM	OVER 20% OF SAMPLE ADHERED TO POUCH AND OUTSIDE OF PAD
NN	PARTICULATES FOUND IN FILTERED SAMPLE
NQ	PART EXCEEDS WHOLE VALUE AND DIFFERENCE IS NOT WITHIN ANALYTICAL PRECISION
	NEGATIVE CALCULATED VALUE IS VALID GIVEN PRECISION OF MEASURED WATER QUALITY PARAMETERS; ACTUAL CALCULATED CONCENTRATION
NV	LIKELY IS LOW; POSSIBLY LESS THAN PQLS OF MEASURED WATER QUALITY PARAMETERS
P	PROVISIONAL DATA
QQ	PART EXCEEDS WHOLE VALUE YET DIFFERENCE IS WITHIN ANALYTICAL PRECISION
R	SAMPLE CONTAMINATED
RR	NO SAMPLE RECEIVED BY LAB FROM FIELD OFFICE
SS	SAMPLE REJECTED DUE TO HIGH SUSPENDED SEDIMENT CONCENTRATION
TP	TORN FILTER PAD
U	MATRIX PROBLEM RESULTING FROM THE INTERRELATIONSHIP BETWEEN VARIABLES SUCH AS PH AND AMMONIA
LID	CONCENTRATION OF FIELD BLANK REFLECTS INITIAL OR ISOLATED OCCURRENCE OF CONTAMINATION; SOURCE OF CONTAMINATION UNDER
UB	INVESTIGATION  For DODOL data, these values are increased and by the second analysis and a 2/07/2000
Un	For DCDOH data, these values are issues or are nulls with no assigned problem codes. 8/27/2008
V	SAMPLE RESULTS REJECTED DUE TO QC CRITERIA  HIGH OPTICAL DENISTY (750 NM); ACTUAL VALUE RECORDED
WW	HIGH OFFICAL DENSITY (750 NW), ACTUAL VALUE RECORDED
X	SAMPLE NOT PRESERVED PROPERLY

#### To Do List

- 1. Data submittal file format changes:
  - WQ\_DATA: add PRECISION\_PC and BIAS\_PC fields
  - WQ\_EVENT: add EVENT\_TYPE and EVENT\_REMARK fields
- Qualify WQP values that are measureable and above the MDL but below the reporting limit using the "G" qualifier code.
- 3. Conduct consistency checks; Provide problem codes as needed (QQ, NQ, IQ, NV).

  Only check consistency of parameters whose values are above the reporting limit.
- 4. Continue reporting replicate (FS1/FS2 or S1/S2) samples.
  - 1. Provide duplicate sample data to three or more significant figures. For low concentrations, submit raw or unrounded data to report 3 figures even if one or two are insignificant.
  - For duplicate sample results failing consistency checks (i.e., NQ), do not null the WQP values, but provide all WQP values.
- 5. Report field blank samples (FB).
  - Assign one of three Problem Codes to any contaminated FB measureable WQP value (>MDL
     on basis of their investigation of the source(s) of contamination (UB, BB, CB).