

#### SeaDataCloud First Training Course Vocabulary Training Session

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First Training, Ostend, 22nd - 27th June 2018 sdn-userdesk@seadatanet.org – www.seadatanet.org



#### Which Vocabularies?

- $\succ$  Parameter Usage Vocabulary (P01)  $\rightarrow$  Focus on this
- ➢ Data Production Tools (L22) →
- > Units of measurement (P06)  $\rightarrow$
- $\succ$  Parameter Discovery Vocabulary (P02)  $\rightarrow$



#### **The P01 Parameter Usage Vocabulary**

- A controlled vocabulary for labelling data channels and data value fields (i.e. recorded parameters, observations and measurement variables in environmental datasets)
- Became a structured compound vocabulary in 2004 supported by a number of semantic models
- The semantic model is the conceptualisation of what is being measured and the management of its constituent parts as separate controlled vocabularies.
- P01 has underpinned BODC data management systems since the 1990s
- Adopted by SeaDataCloud and more recently by OBIS (De Pooter et al, 2017 <u>https://doi.org/10.3897/bdj.5.e10989</u>) to facilitate data exchange, interoperability and discovery

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#### **BODC P01 collection**

← → C A Natural Environment Research Council [GB]   https://www.bodc.ac.uk/resources/vocabularies/vocabulary_search/P01/				
NVS editor NVS vocabulary builder BODC parameter	Search text Conc	entration of % Vocabulary P01, BODC Parameter Us advanced	options Search	
codes SeaVoX	Found 12533 reco	rds   Show ( 11 - 20 )     <u>« First   Prev</u>   <u>1</u> 2 <u>3</u> <u>4</u> <u>5</u> <u>6</u> <u>7</u> <u>Next &gt;</u> <u>Last »</u>	<u>download results</u>   <u>s</u>	<u>tart again</u>
Delivery formats	▲ Identifier ▼	▲ PrefLabel ▼	▲ Definition ▼	▲ Date
<ul> <li>Products</li> <li>Help and hints</li> <li>Portals and links Search</li> </ul>	FA63GCP1	Concentration of methyl hexatriaconta-7E,14E,21E-trienoate {C36:30 methyl ester} per unit volume of the water body [particulate >GF/F phase] by filtration and gas chromatography-mass spectrometry	Gas chromatography mass spectromtry (GF/F filtered)	2018- 02-27
	ME82GCP1	Concentration of octatriaconta-16E,23E-dien-2-one {C38:2 methyl ketone} per unit volume of the water body [particulate >GF/F phase] by filtration and gas chromatography-mass spectrometry	Gas chromatography mass spectromtry (GF/F filtered)	2018- 02-27
	ME83GCP1	Concentration of octatriaconta-9E,16E,23E-trien-2-one {C38:3 methyl ketone} per unit volume of the water body [particulate >GF/F phase] by filtration and gas chromatography-mass spectrometry	Gas chromatography mass spectromtry (GF/F filtered)	2018- 02-27
	ESTSED13	Concentration of methyl 2-hydroxy hexadecanoate per unit dry weight of sediment	The amount (mass or moles) of the specified organic compound per unit mass of dry sediment.	2018- 02-27
	ESTSED14	Concentration of methyl 2-hydroxy heptadecanoate per unit dry weight of sediment	The amount (mass or moles) of the specified organic compound per unit mass of dry sediment.	2018- 02-27
	ESTSED15	Concentration of methyl 2-hydroxy docosanoate {behenic acid methyl ester CAS 929-77- 1} per unit dry weight of sediment	The amount (mass or moles) of the specified organic compound per unit mass of dry sediment.	2018- 02-27
1 -		Concentration of methyl 2-hydroxy tetracosanoate {CAS 2433-95-6} per unit dry weight	The amount (mass or moles) of the	2018-







## **Conceptual model criteria**

- Standardisation with minimum loss of information
- Consistency
- Unambiguous names and definitions
- Meaningful to the human user

#### BUT

- Semantic rigour necessary to enable machine interpretation
- Enablement of automated processes must come first
- Interoperability by application of Semantic Web standards and mapping to authoritative vocabulary digital resources.



#### How to find a P01 parameter code?

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# How to find a P01 parameter code?

- 1. Understand the BODC semantic models including components, structure and logic
- 2. Analyse what you are trying to map and match to the P01 semantic structure
  - 1. What is the object of interest?
  - 2. What is the property?
  - 3. What is the matrix?
- 3. Search using your favourite tool or a combination of online tools
- 4. Use match on external identifiers such as CAS numbers or CheBi IDs or Aphia IDs or ITIS TSN when appropriate
- 5. This is not easy
  - scientific measurements are complex and extremely diverse
  - attempt to model them can be subjective
  - Optimise for machine-to-machine communication
  - Errors are made so provide feedback by email to vocab.services@bodc.ac.uk



## **Understand the semantic models**

- The Parameter semantic model
  - The Measurement Matrix semantic model
    - Matrix for Physical entities
    - Matrix for other entities
  - The Biological entity semantic model



## **The Parameter semantic model**



#### Parameter semantic model - 3 main elements





#### Parameter semantic model - all component elements





#### **Examples**



reactive particulate]

**Concentration standard deviation of ammonium {NH4+ CAS 14798-03-9} per unit mass of the water body** [dissolved plus reactive particulate]

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### **Rigorous semantics**

- 1) The parameter entity (i.e. property of interest) = a quantitative or nominative property of an object of interest
- 2) The object of interest = a chemical, biological or physical entity;
- 3) The matrix = the environmental entity to which the chemical, biological or physical entity relates or in which it is embedded;
- The statistical entity allows us to create separate concepts for any statistical parameters associated with the measured property (e.g. standard deviation, uncertainty, standard error, annual mean, etc.).
- If the statistical parameter is set to "not specified" then the reported property is the parameter entity (e.g. "Concentration");
- If it is specified then the reported property is the statistical parameter of the parameter entity (e.g. "Concentration standard deviation")



## The Parameter semantic model vocabularies







#### **The MATRIX semantic model**





#### **The MATRIX semantic model**





# The Biological Entity semantic model





# Mapping the source parameter to a P01 code – key questions

- 1. What is the object of interest?
- Is it a chemical substance? A biological entity? A physical entity? Not sure?
- 3. What kind of quantity or property was measured or reported?
- 4. In what environment or on what substrate was the observation made?
- 5. How is the measurement reported? What basis was used? what units?
- 6. How was the measurement made?
- 7. Was the sample filtered? If so what was the pore size or filter type?
- 8. Does the object of interest need to be sub-setted into classes like for example electromagnetic radiation wavelengths or particle size-classes?



## Search Tools

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#### **Hierarchical search**

- Drill down P08 > P03 > P02 > P01
- <u>http://seadatanet.maris2.nl/v bodc vocab v2</u> /vocab relations.asp?lib=P08
- Best for
- exploring / browsing parameter discovery terms
- inexperienced user to get a feel for the classification of parameter codes



# Keyword search using the BODC Vocab Search tool

- https://www.bodc.ac.uk/resources/vocabularies/vocabulary\_search/p01/
- e.g. search for Concentration%chlorophyll-a%water body%spectrophotometry
- Best for

- experienced users who know the P01 parameter dictionary and its semantic models

- Main advantages:
- can search on the identifier, the preferred label, the alternative label or the definition
- displays the definitions on the screen
- Option to output full record of selected parameter to a file
- Ink to full record and mappings. This is an easy way to find the PO2 group code associated with a PO1 code for example.



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#### Semantic component facet search using the MARIS tool http://seadatanet.maris2.nl/bandit/browse\_step.php

- Best for users who are not very familiar with the P01 parameter dictionary and its semantic construction
- Start with a keyword then drill down the list of possible codes selecting terms relevant to the search
- e.g. start by entering chlorophyll-a in the search box select concentration P02= Chlorophyll pigment concentrations in water bodies select the appropriate matrix (e.g. water body [particulate >GF/F phase]) the analytical method if wanted (e.g. HPLC)



# Search and submit using the BODC Vocab Builder tool

- <u>https://www.bodc.ac.uk/resources/vocabularies/vocabulary\_buil\_der/</u>
- Can be used as a search tool if not logged in
  - or search and submit if logged in
- Best for
- - exploring biological entity, matrix and parameter semantic models
- - experienced users who want to submit a new P01 code, a new biological entity or a new matrix code or any new terms related to any of these models



<ul> <li>Inventories</li> <li>Vocabularies</li> </ul>	P01 Chemical Entity Parameter Code Builder
NVS search tool NVS editor NVS vocabulary builder BODC parameter codes SeaVoX	Preferred label Concentration of chlorophyll-a {chl-a CAS 479-61-8} water body [particulate >GF/F phase]
<ul> <li>Delivery formats</li> <li>Products</li> <li>Help and hints</li> </ul>	show/hide exact results   reset all
<ul> <li>Portals and links</li> <li>Search</li> </ul>	Found 17 exact matches
	✓ Select a measurement property
700	Select a measurement statistical qualifier
States A	✓ Select a chemical substance
· · · · · · · · · · · · · · · · · · ·	Select a measurement-matrix relationship
	✓ Select a matrix
all and the second s	Destruction for factors

#### Return to index

Login to enable new concept creation

Antarctic Peninsula ©



# Subjectivity examples

Submitted as:

"Concentration of tar per unit dry weight of sand by sieving and gravimetry" Became:

"Dry weight of tar residues per unit area of the sediment by sieving, picking and gravimetry"

Biota entries:

"Number Phoronida (brachiopod larvae)"

Became

"Abundance of Brachiopoda (ITIS: 156755: WoRMS 1803) [Stage: larvae] per unit volume of the water body by optical microscopy"

P01=ABR08136



# MARIS DEMO 1

# Using the MARIS facet search tool http://seadatanet.maris2.nl/bandit/browse\_step.php Find:

Chlorophyll-a extracted from a water sample, filtered on GF/F, extracted in acetone, analysed by fluorometry and expressed in micrograms per litre



# MARIS DEMO 1

Main keyword=Chlorophyll-a > enter in input string box

Property > concentration

- Matrix > water body [particulate >GF/F phase]
- Analytical method > fluorometry

Sample preparation > filtration, acetone extraction

Measurement-Matrix relationship > per unit volume of the



# BODC DEMO 1

Use the BODC keyword search tool
https://www.bodc.ac.uk/resources/vocabularies/vocabulary\_search/p01/

Use the Advanced search

Find:

Chlorophyll-a extracted from a water sample, filtered on GF/F, extracted in acetone, analysed by fluorometry and expressed in micrograms per litre



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# BODC DEMO 1

## Concentration of%chlorophyll-a%per unit volume%water body%>GF/F%acetone%fluorometry%



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#### Be Aware

Ensure use of the "%" as a wildcard

Use the wildcard to account for the plural forms

• A P01 Label always starts with an Upper case

• The spelling is British English spelling



# Using the BODC Vocab Builder

### https://www.bodc.ac.uk/resources/vocabularies/vo cabulary\_builder/

#### P01 Chemical Entity Parameter Code Builder

-Preferred label-

Concentration not specified of chlorophyll-a {chl-a CAS 479-61-8} per unit volume of the water body [particulate >GF/F phase]

show/hide exact results | show/hide close match results | reset all

Found 13 exact matches | Showing (1 - 10) | 1 2 Next Last

# Submit New BODC Code DEMO 1

You need a standard deviation code for:

Concentration of chlorophyll-a {chl-a CAS 479-61-8} per unit wet volume of sediment by acetone extraction and spectrophotometry

http://vocab.nerc.ac.uk/collection/P01/current/CO CHSE04/

Concentration of chlorophyll-a {chl-a CAS 479-61-8} per unit wet volume of sediment by acetone extraction and spectrophotometry

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Additional Mappings ICES Codes to BODC P01 ICES: <u>http://vocab.ices.dk/</u> PARAM:SPECI:MATRX:SEXCO:BASIS HG:Pleuronectes platessa: LI: F: W Mercury:127143:Liver:Female:Wet weight

#### BODC = HGMMCF21

Concentration of mercury {Hg} per unit wet weight of biota {Pleuronectes platessa (ITIS: 172902: WoRMS 127143) [Sex: female Subcomponent: liver]}

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# Examples – MARIS and BODC

#1 Exercise to practice selection of complex matrix/phases

Find the P01 and P02 codes for a dataset containing sizefractionated chlorophyll-a extracted in acetone and analysed by fluorometry reported in µg/l for the following size fractions:

- 1. 0.2-2,
- 2. 2-20,
- 3. 20-200
- 4. >0.2 microns obtained by summing the concentrations in the size-fractions.

# Examples – MARIS and BODC

#2 Exercise to practice finding a suite of related measurements and illustrate use of synonyms or multiple accepted spellings.

Find the P01 and P02 codes for parameters associated with an HPLC pigment speciation dataset. The pigments to be mapped are chl-a, divinyl chlorophyll-a, alpha-carotene, and pheophytin a. The samples were filtered on 0.2um nuclepore membrane, extracted in acetone, analysed by HPLC reported in units of micrograms and picograms per litre.



# Examples – MARIS and BODC

#3 Exercise

Find the P01 and P02 codes for chlorophyll concentrations measured using an in situ fluorometer deployed on a CTD profiling package

#### #4 Exercise

Find the P01 and P02 codes for a nutrient dataset for silicate, nitrate plus nitrite, nitrite, phosphate concentrations measured on unfiltered water samples



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#### Answers

#### #1 Exercise

- http://vocab.nerc.ac.uk/collection/P01/current/SCHLFLPF/
- http://vocab.nerc.ac.uk/collection/P01/current/SCHLFLPG/
- http://vocab.nerc.ac.uk/collection/P01/current/SCHLFLPH/
- http://vocab.nerc.ac.uk/collection/P01/current/CPHLFLP4/
- http://vocab.nerc.ac.uk/collection/P02/current/CPWC/

#### Answers

#### #2 Exercise

**Tip**: if using the BODC search tool, list the 61 pigment category types corresponding to concentration per unit volume of the water body [particulate >0.2um phase] by filtration, acetone extraction and high performance liquid chromatography (HPLC); then select the appropriate one from that by scrolling down or extracted to a file.

http://vocab.nerc.ac.uk/collection/P01/current/CPHLHPP5/ P02=CPWC http://vocab.nerc.ac.uk/collection/P01/current/ACARHPP5/ or http://vocab.nerc.ac.uk/collection/P01/current/BECAHPP5/ P02=CARO http://vocab.nerc.ac.uk/collection/P01/current/DVCAHPP5/ P02=CPWC http://vocab.nerc.ac.uk/collection/P01/current/PTAXHPP5/ P02=PHWC



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#### Answers

#### #3 Exercise

**Tip**: if using the BODC Vocab search tool use the additional filter to exclude anything that contains extraction. This gives you 25 returns. Simply scrolled down the list to find the one that fits your data.

In this case the preferred option is to go for the generic code for in situ fluorometer data:

http://vocab.nerc.ac.uk/collection/P01/current/CPHLPR01/



#### Answers

#4 Exercise (N.B. 2<sup>nd</sup> option is the wider option) <u>http://vocab.nerc.ac.uk/collection/P01/current/SLCAMS01</u> P02=SLCA Or <u>http://vocab.nerc.ac.uk/collection/P01/current/SLCAZZXX/</u> P02=SLCA

http://vocab.nerc.ac.uk/collection/P01/current/NTRZYYDZ P02=NTRA Or http://vocab.nerc.ac.uk/collection/P01/current/NTRZZZXX/ P02=NTRA

http://vocab.nerc.ac.uk/collection/P01/current/NTRIYYDZ P02=NTRI Or http://vocab.nerc.ac.uk/collection/P01/current/NTRIZZXX/ P02=NTRI

http://vocab.nerc.ac.uk/collection/P01/current/PHOSYYDZ P02=PHOS Or http://vocab.nerc.ac.uk/collection/P01/current/PHOSZZXX/ P02=PHOS