

The classification of metals and sparingly soluble metal compounds

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**Eurometaux
Environmental Classification workshop
March 6, 2009**

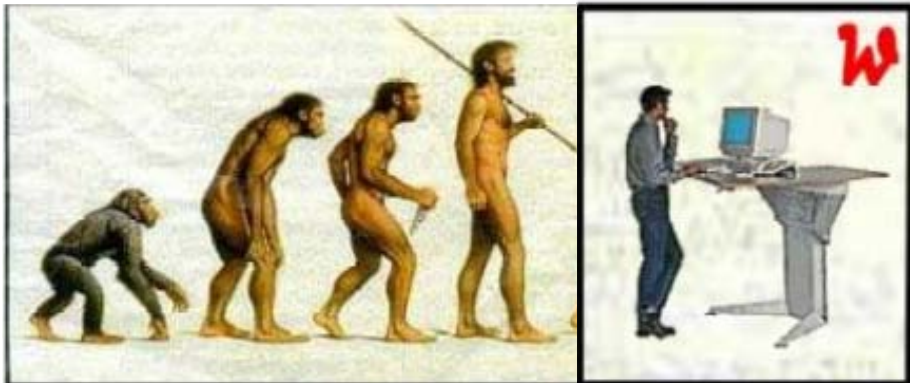


At the beginning of time....



- Classify a metal according to the toxicity of its soluble salt

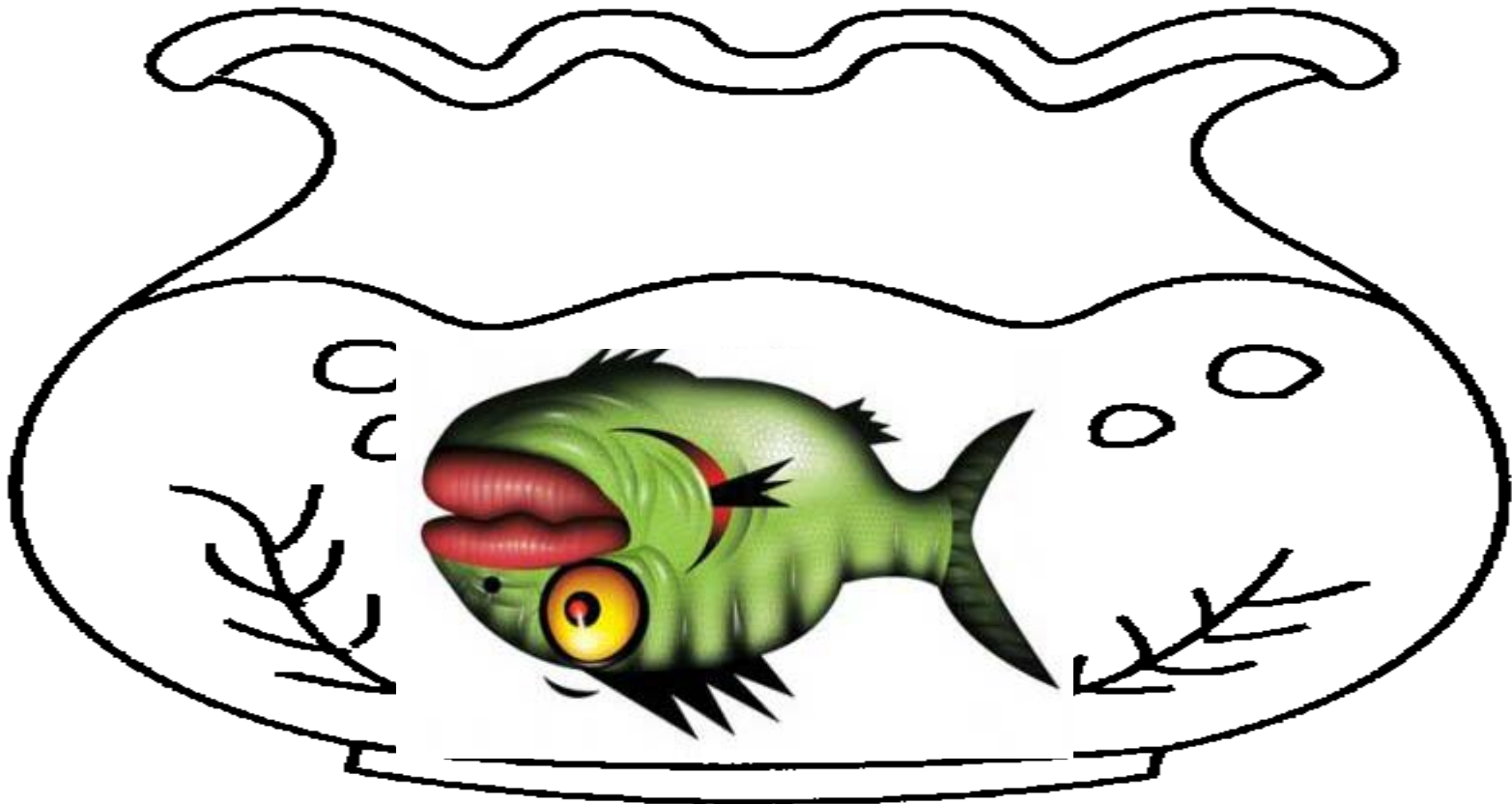
- Problems in classifying insoluble metals, sparingly soluble metals and massives



- Rate and extent of metal transformation to the bioavailable form is key to its hazard identification

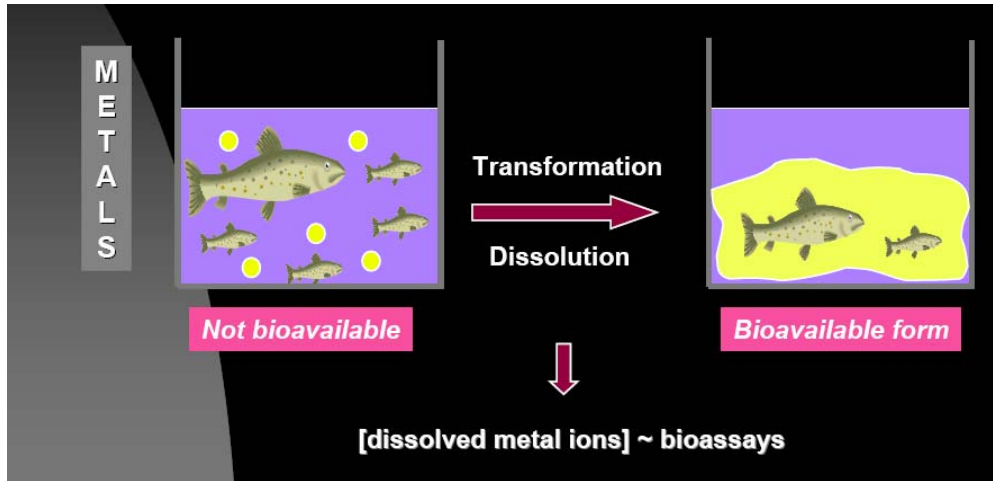


Transformation/dissolution



Transformation/dissolution (T/D) tests- OECD protocol

Test principle



Test design

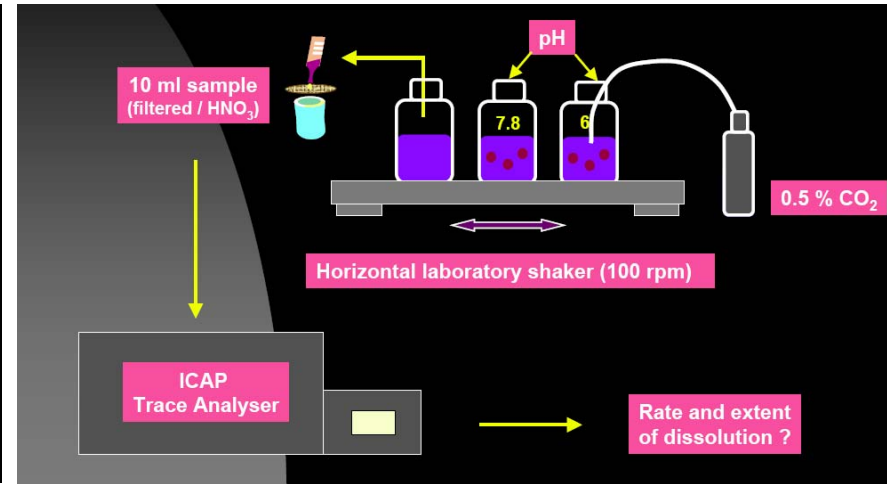
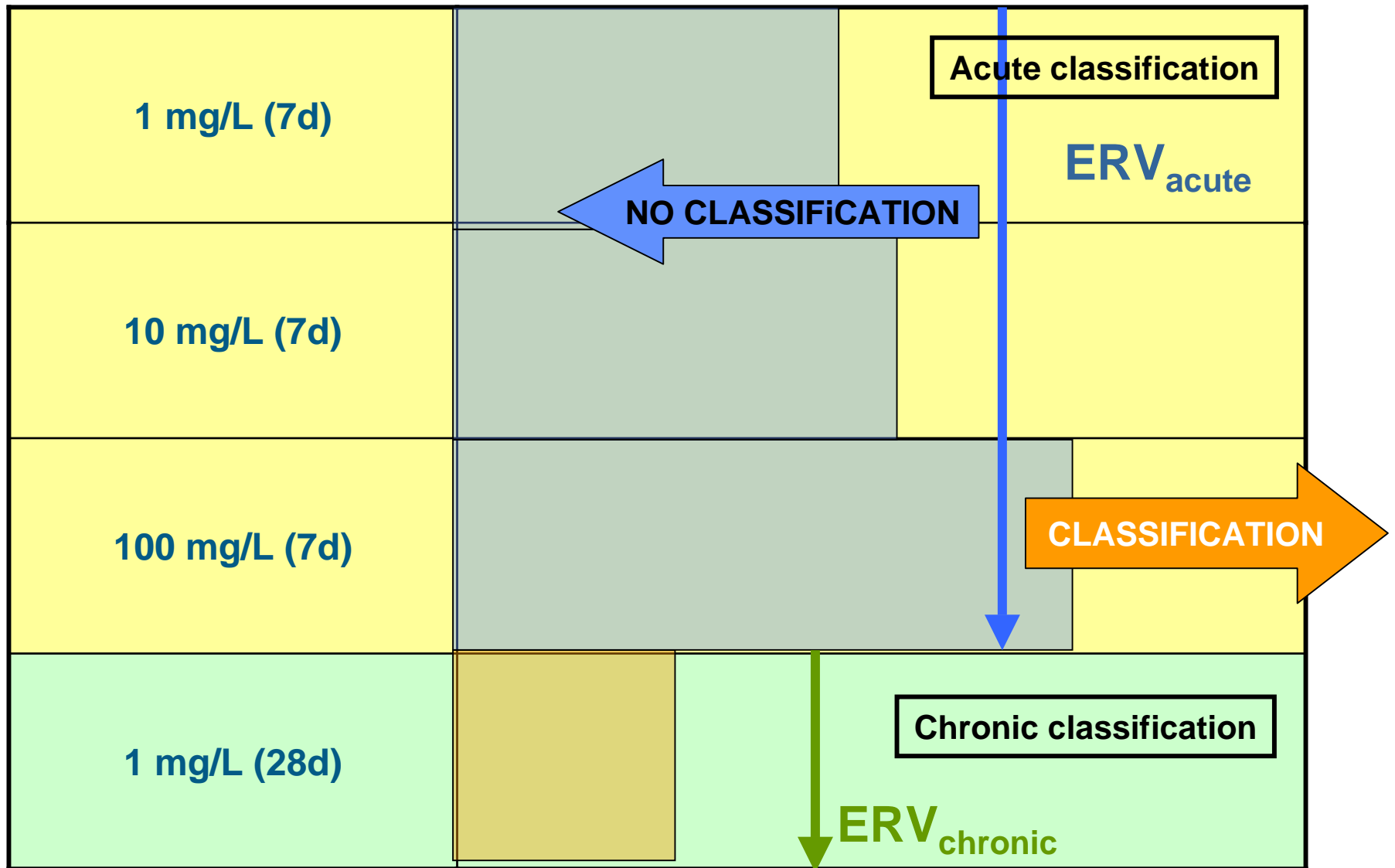


Figure from LISEC

- ❑ Exposure time: 7 days (acute); 28 days (chronic)
- ❑ SS metal compounds and metals (powders, massives)
- ❑ Shaking: 100 rpm, without causing abrasion
- ❑ Exposure medium: OECD 203 modified, pH 6, 7 & 8

Cut off points (acute and chronic classification)

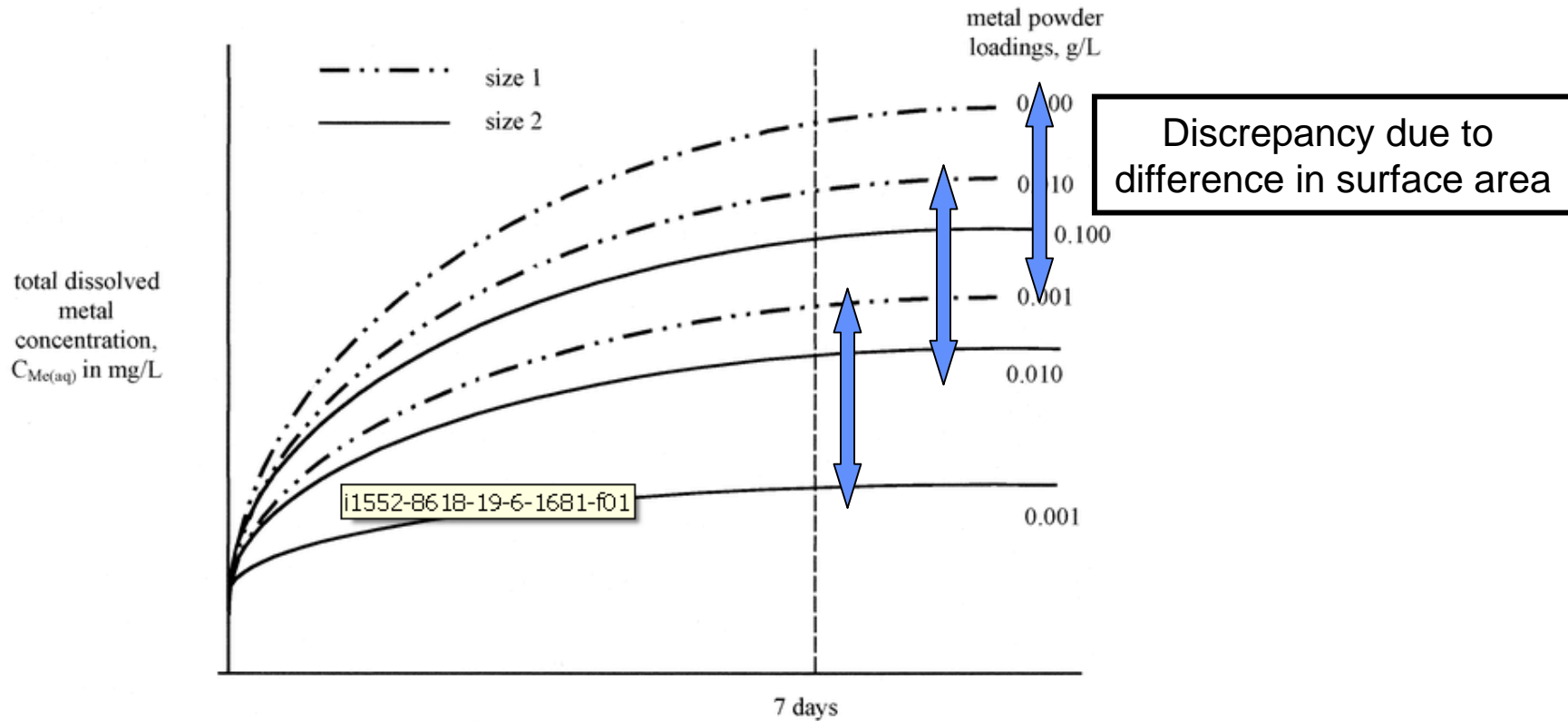


What to test with T/D ??

Type	Particle size	Comments
Metal compounds	Smallest representative size sold	Never larger than 1 mm
Metals – powders	Smallest representative size sold	May need to consider different sources if yielding different crystallographic / morphologic properties
Metals – massive	1 mm	Default value may be altered if sufficient justification

Annex 10 (GHS) mentions "As in addition the surface area of the particles in the test sample has an important influence on the rate and extent of transformation/dissolution, **powders are tested at the smallest representative particle size as placed on the market, while massives are tested at a particle size representative of normal handling and use.** A default diameter value of 1 mm should be used in absence of this information. For massive metals, this default may only be exceeded when sufficiently justified. The specific surface area should be determined in order to characterize and compare similar samples"

T/Dp tests results: size matters!

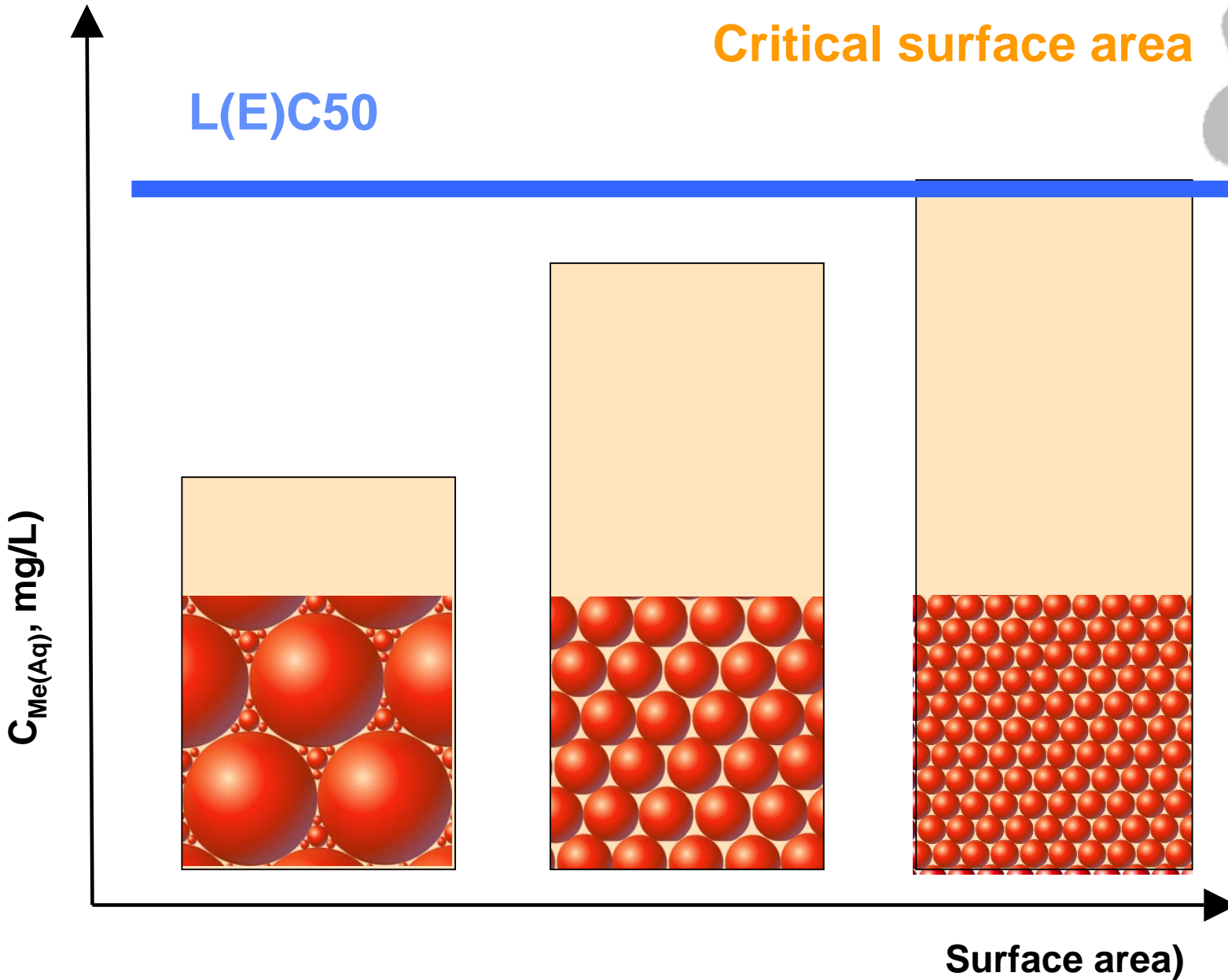


- Conduct experiments according to a standardized transformation protocol to establish the concentration of total dissolved metal, $C_{Me(aq)}$ in mg/L, as a function of time in a specified aqueous test medium of composition comparable to those used in conventional aquatic toxicity testing.
- Reaction kinetics of two particle sizes of a hypothetical metal powder at three loadings in an aqueous medium, schematic basis

Differences in surface area

L(E)C50

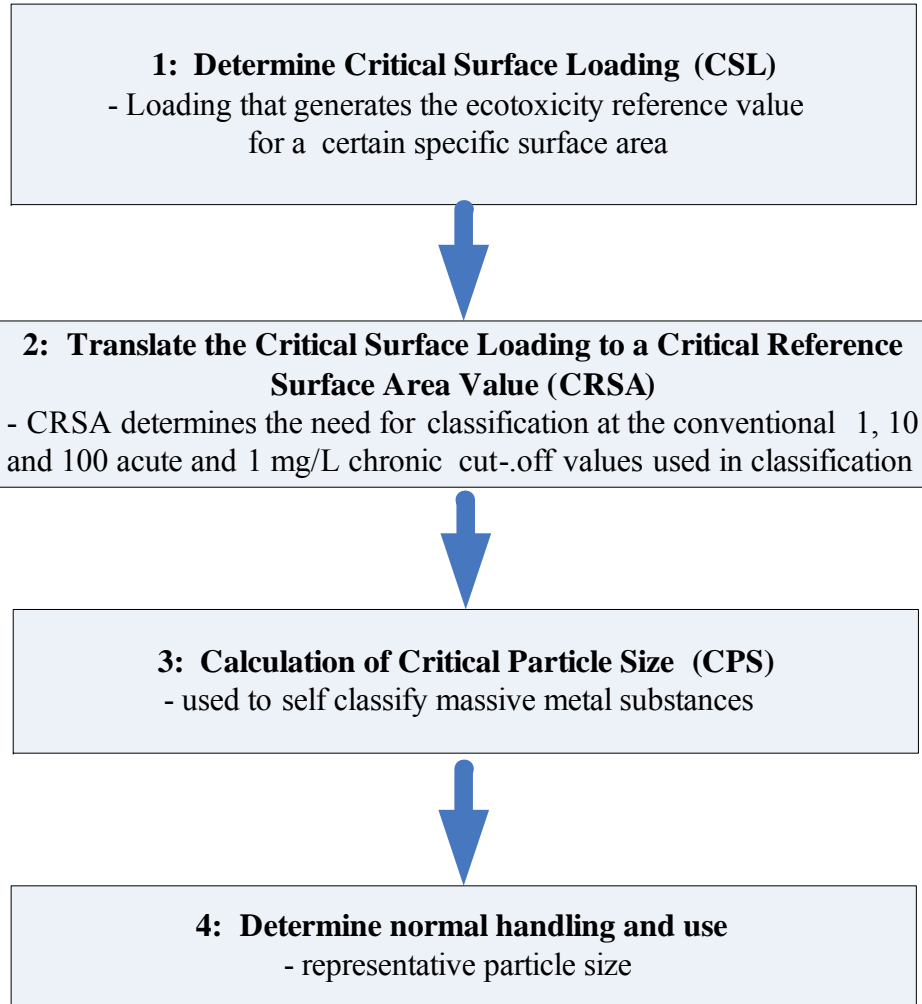
Critical surface area



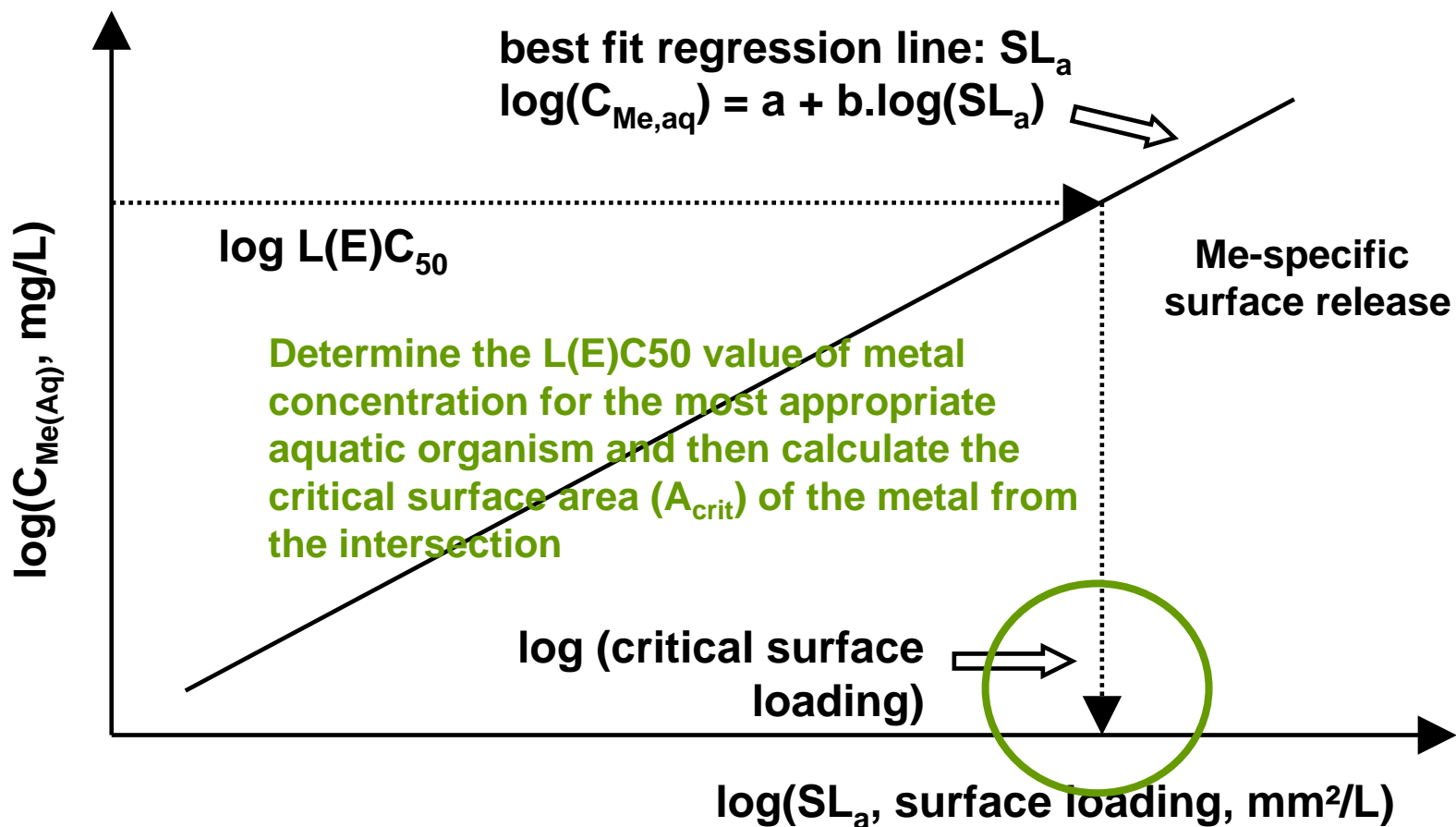
Critical surface approach/critical particle Size concept

- enables self classification for massives, powders
- Originally developed for metals and sparingly soluble metals, but can be extended to alloys
- Concept based on establishing a correlation between dissolved metal concentration (measured in T/Dp) after a specified time interval and the surface area loadings
- Critical Surface Area: surface area that will generate the ecotoxicity reference value (e.g. LC50) after a certain time period
- Critical Particle Size : particle size that will generate the ecotoxicity reference value (e.g. LC50) after a certain time period
- Critical Diameter (CD): diameter from a spherical particle that will generate the ecotoxicity reference value after a certain time period (standardization)

Steps critical surface approach/critical particle Size concept



Step 1: Determine critical surface loading



surface area loading (A , mm^2/L) = substance specific surface area (SA , m^2/g) * substance mass loading (g/L)



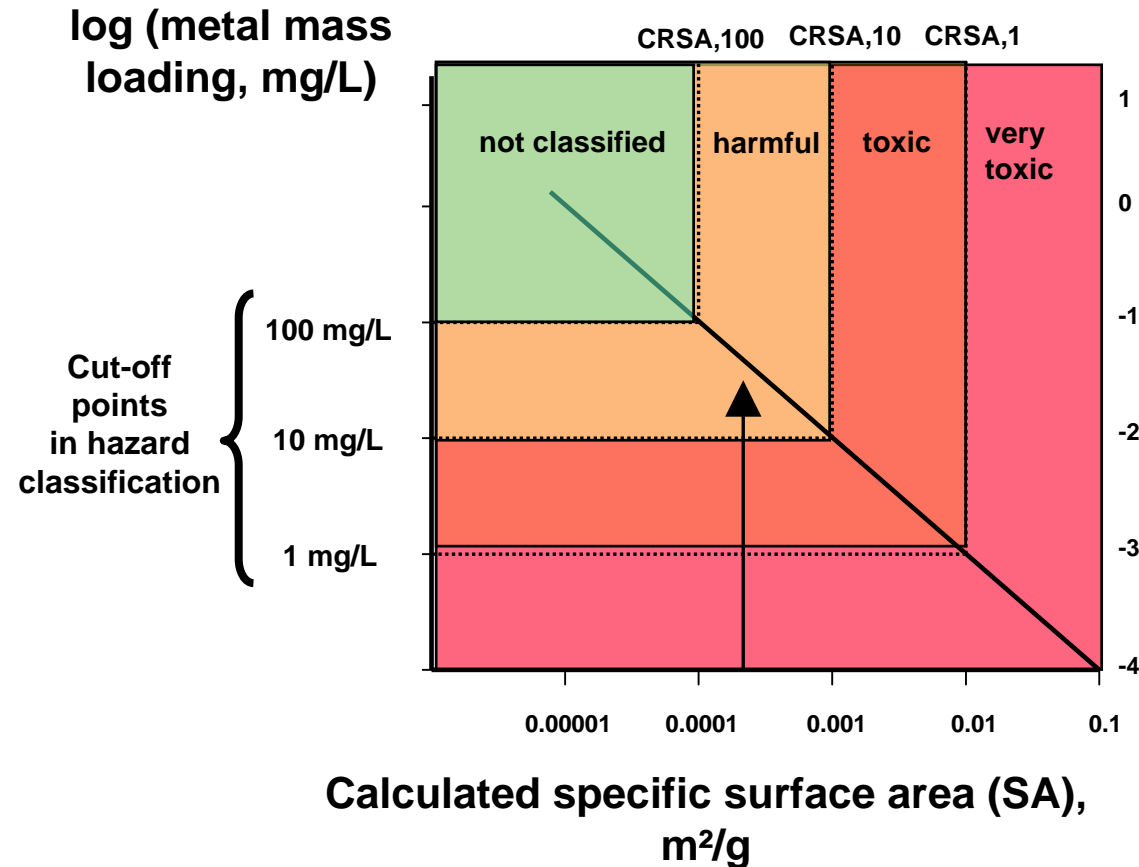
$SA = \text{area (m}^2\text{)}/\text{mass (g)}$



1, 10, 100 mg/l

Calculation of the single hazard identification line & self classification

$$SA_{cp, crit} (m^2/g) = A_{crit} (mm^2/l) / 10^3 cp (mg/l)$$



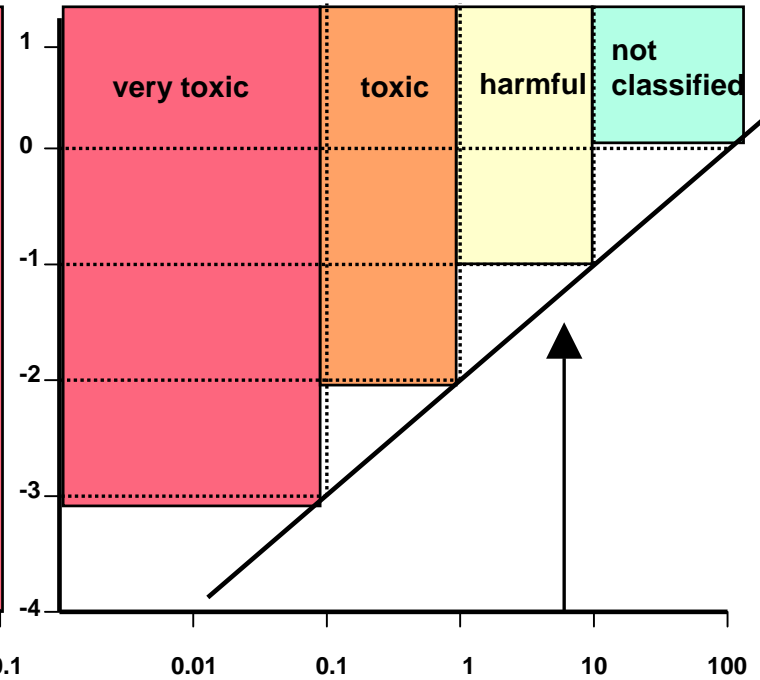
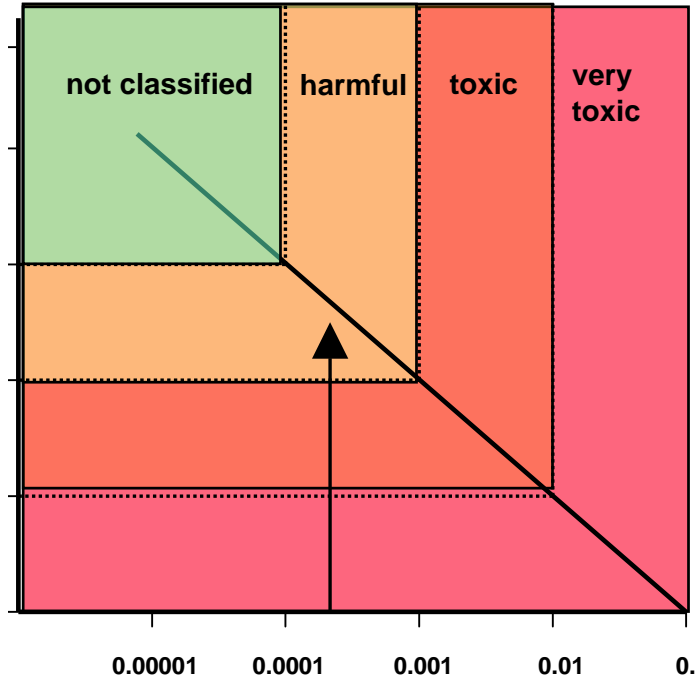
For each of the standard 100-, 10-, and 1-mg/L cut off points, cp, used in hazard classification, there will be a critical specific surface area, $SA_{cp, crit}$, in m²/g, that delivers the L(E)C50 to the aqueous medium

Critical diameter

log (metal mass loading, mg/L)

CRSA,100 CSRA,10 CRSA,1

CD,1 CD,10 CD,100



Calculated specific surface area (SA),
m²/g

Metal particle diameter (D), mm

$$D_{cp,crit} \text{ (mm)} = \frac{6}{SA_{cp,crit} \text{ (m}^2\text{/g)} \cdot \text{density (g/cm}^3\text{)} \cdot 10^3}$$

Overview classification strategy metal/metal compounds

1: Evaluation solubility -metal compounds

- Estimated from solubility product
- Transformation/dissolution protocol



2: Application of Critical Surface Approach concept - massives/powders

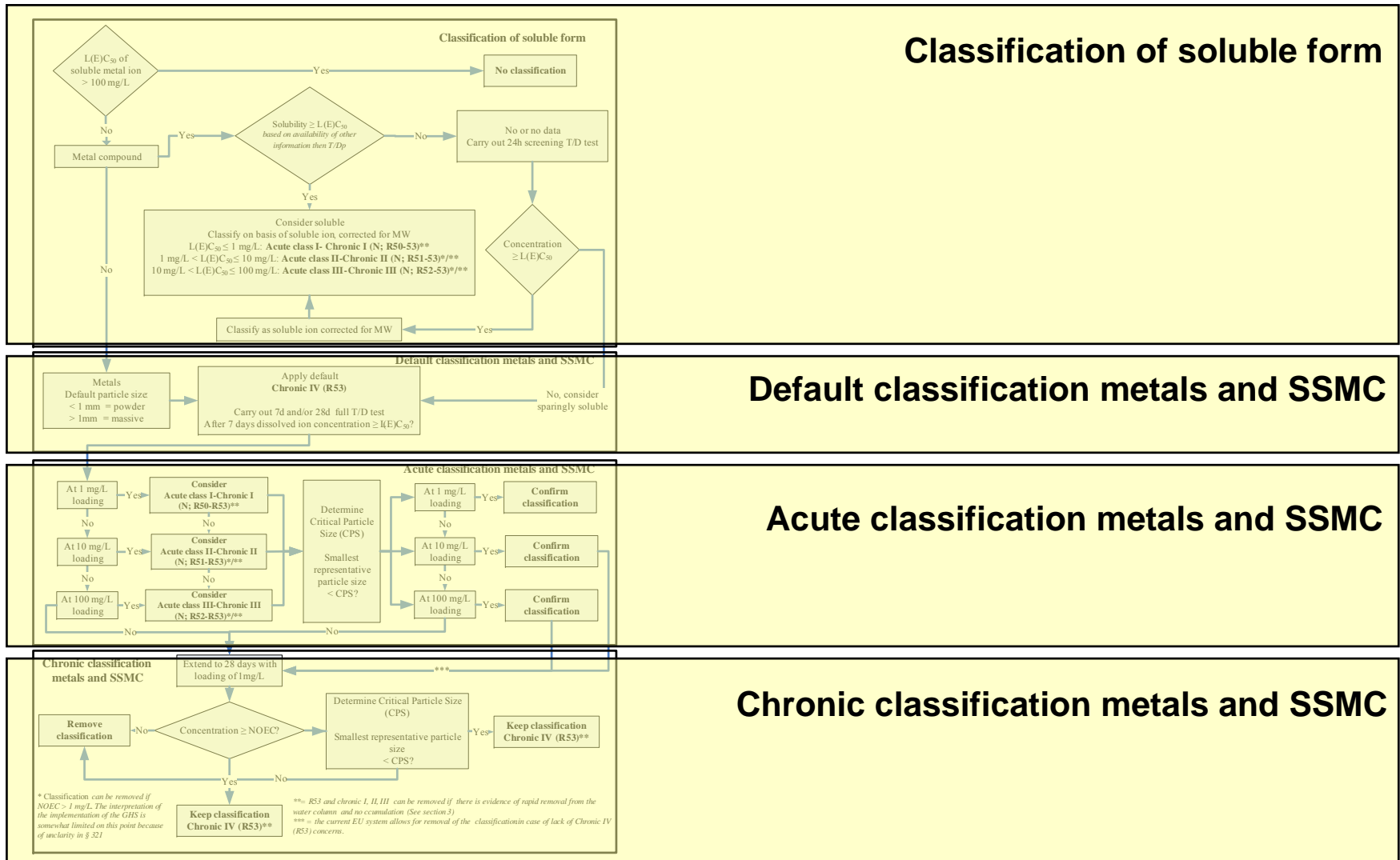
- default diameter value of 1 mm



3: Calculation of Critical Particle Size -massives/powders

- comparison with normal handling and use

Classification strategy metal/metal compounds



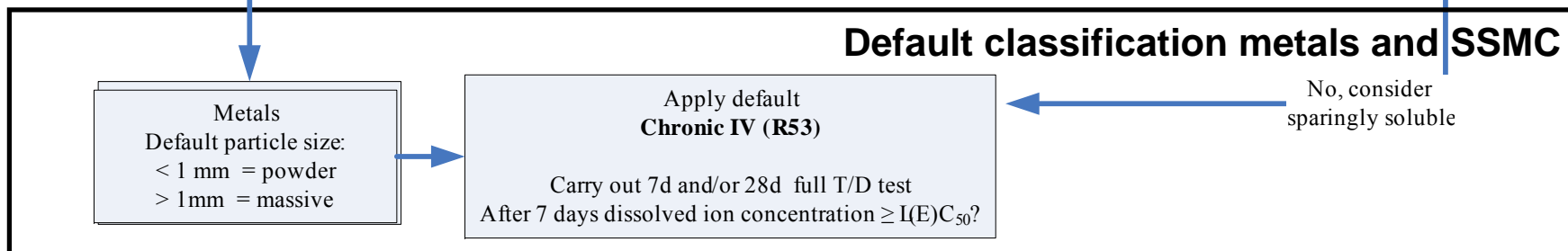
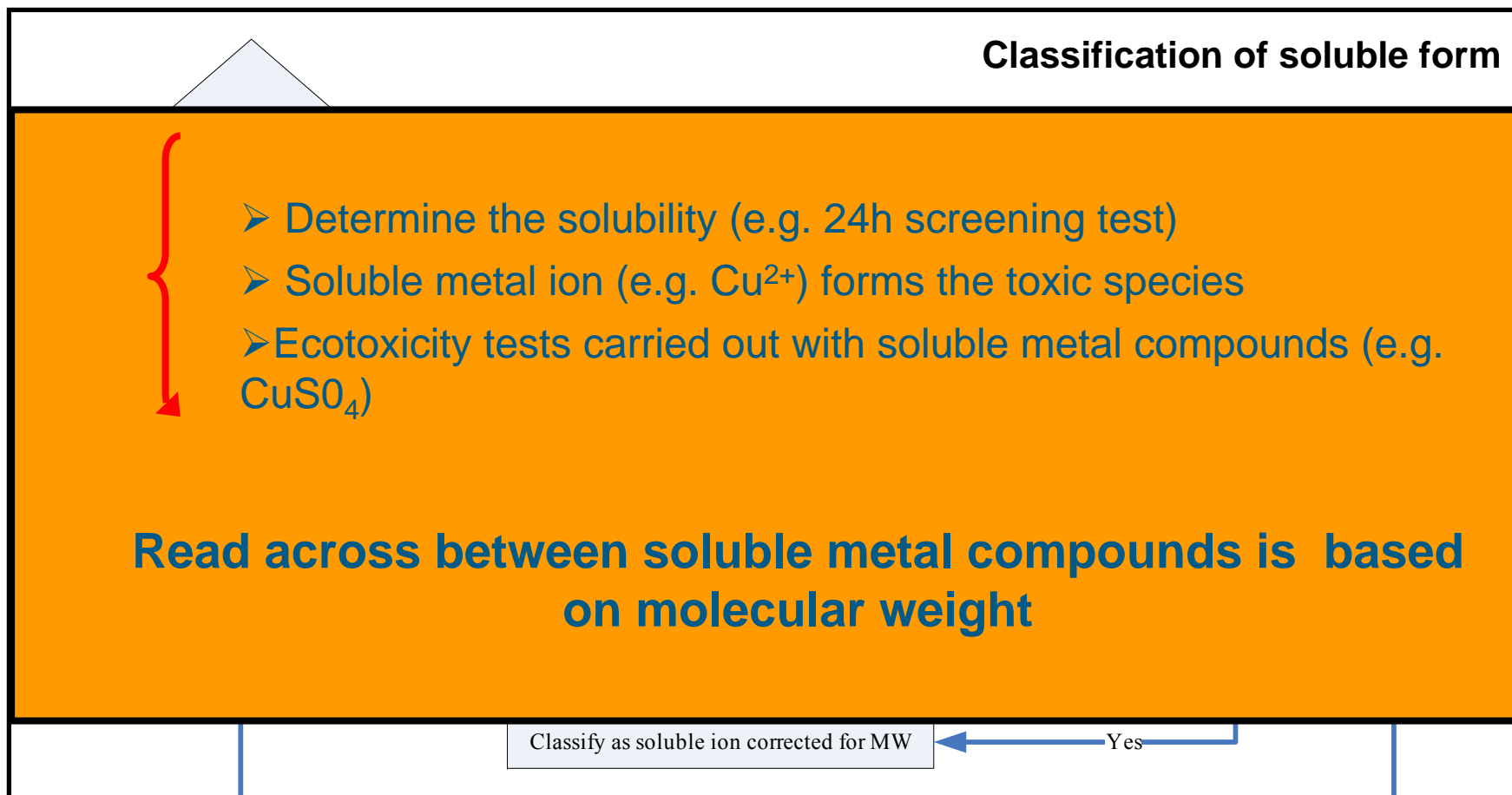
Classification of soluble form

Default classification metals and SSMC

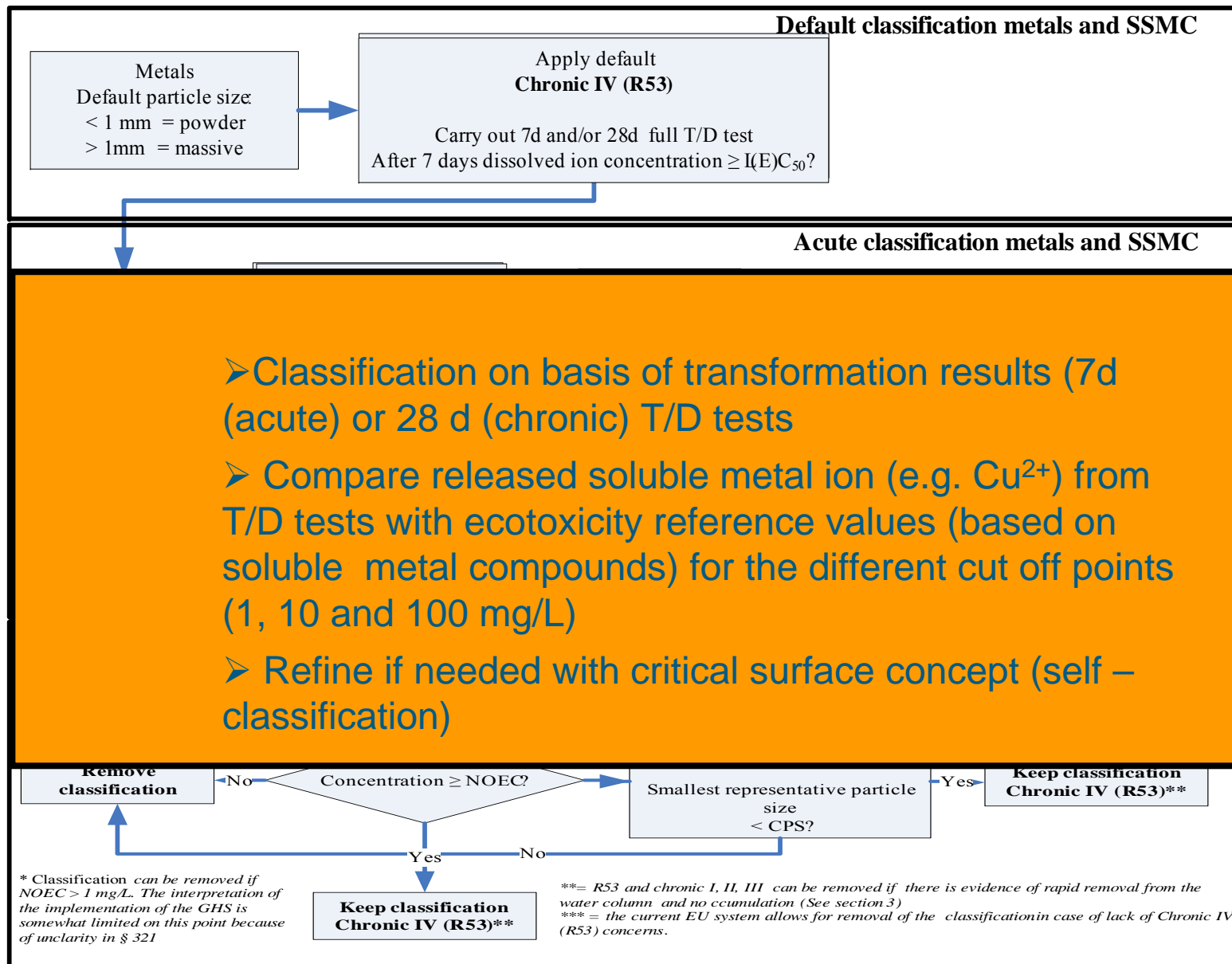
Acute classification metals and SSMC


Chronic classification metals and SSMC

Classification strategy metal/metal compounds (A)



Classification strategy metal/metal compounds (B)

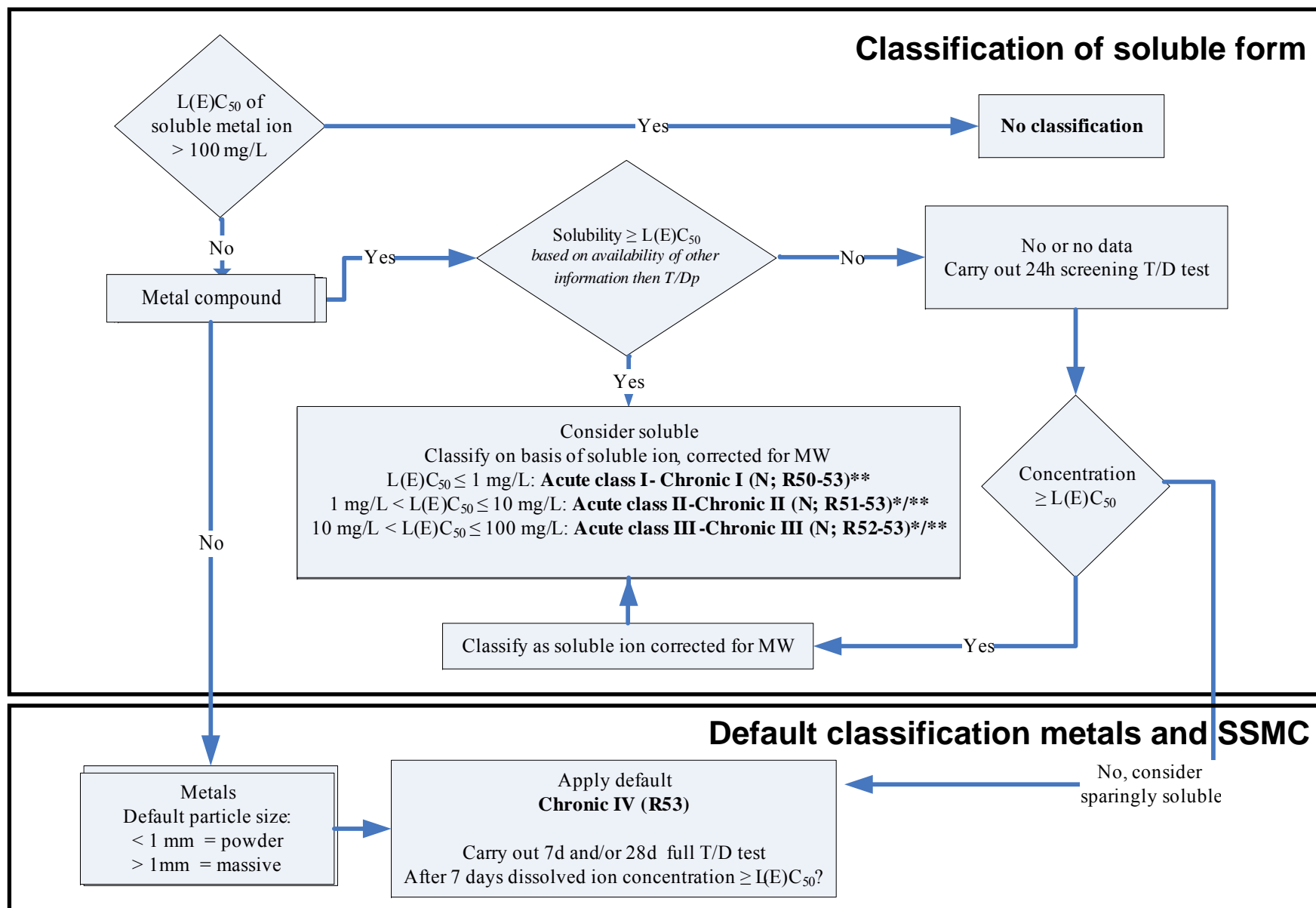


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- application to alloys : Jim Skeaff
 - Practical examples: this afternoon

**THANKS
FOR YOUR
ATTENTION**



Classification strategy metal/metal compounds (A)



Classification strategy metal/metal compounds (B)

