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## Experimental data annotation guided by an ontology for decision support: @Web project

Patrice Buche, Juliette Dibie

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# Experimental data annotation guided by an ontology for decision support: @Web project

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# L'équipe projet @Web en 2014

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# Heterogeneous data reuse for decision support

(Destercke et al. 2011, Buche et al 2013, Destercke et al. 2013, Tamani et al. 2014, Guillard et al. 2015)



- Scientific advances



- Food quality



- Consumer safety

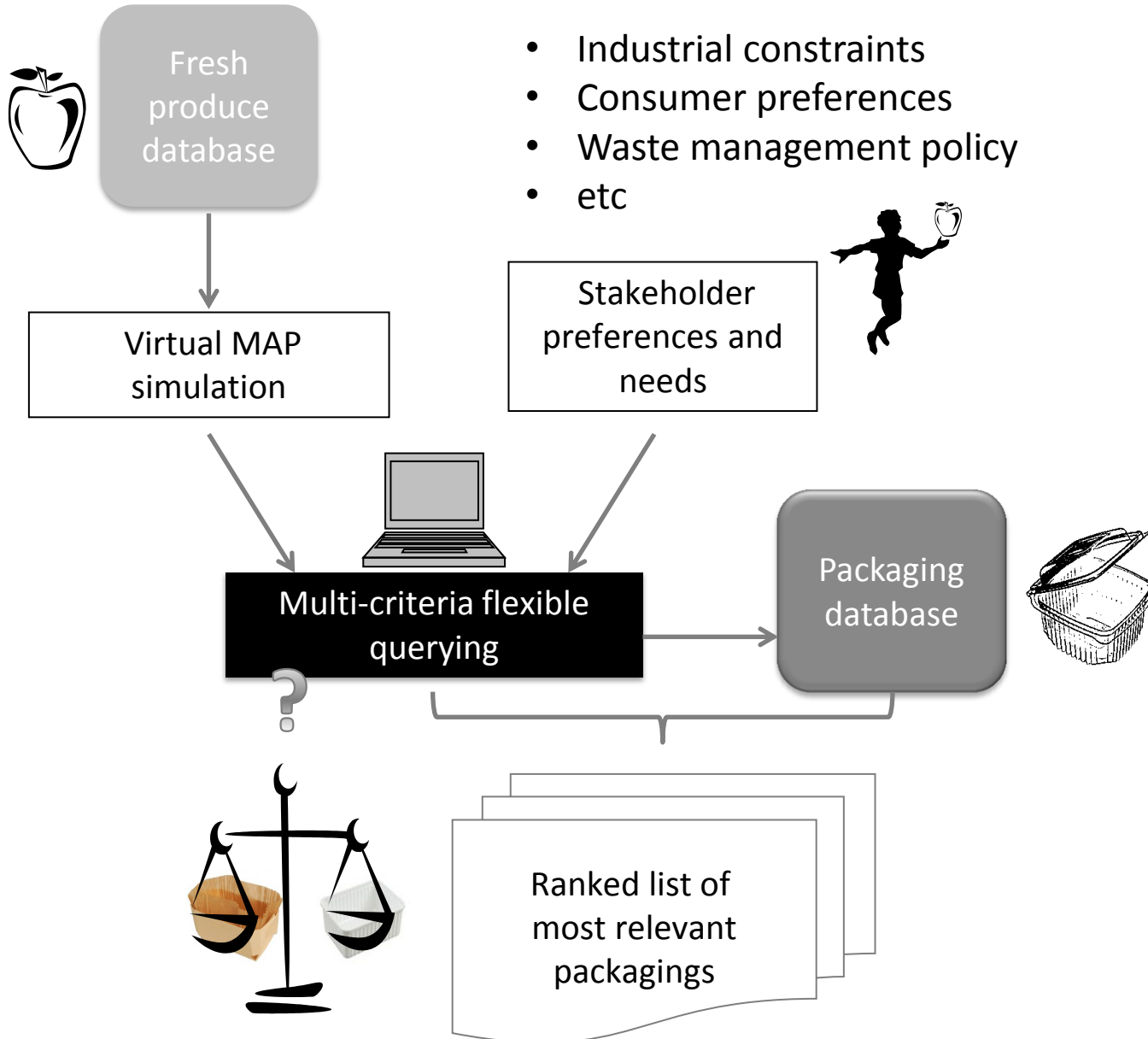
- Economical competitiveness



- Environmental protection



*I want a packaging which preserves my product, made of renewable resources, but without GMO, if possible transparent and with a « material » cost < 3 € / kg ...*



- Industrial constraints
- Consumer preferences
- Waste management policy
- etc

Virtual MAP simulation

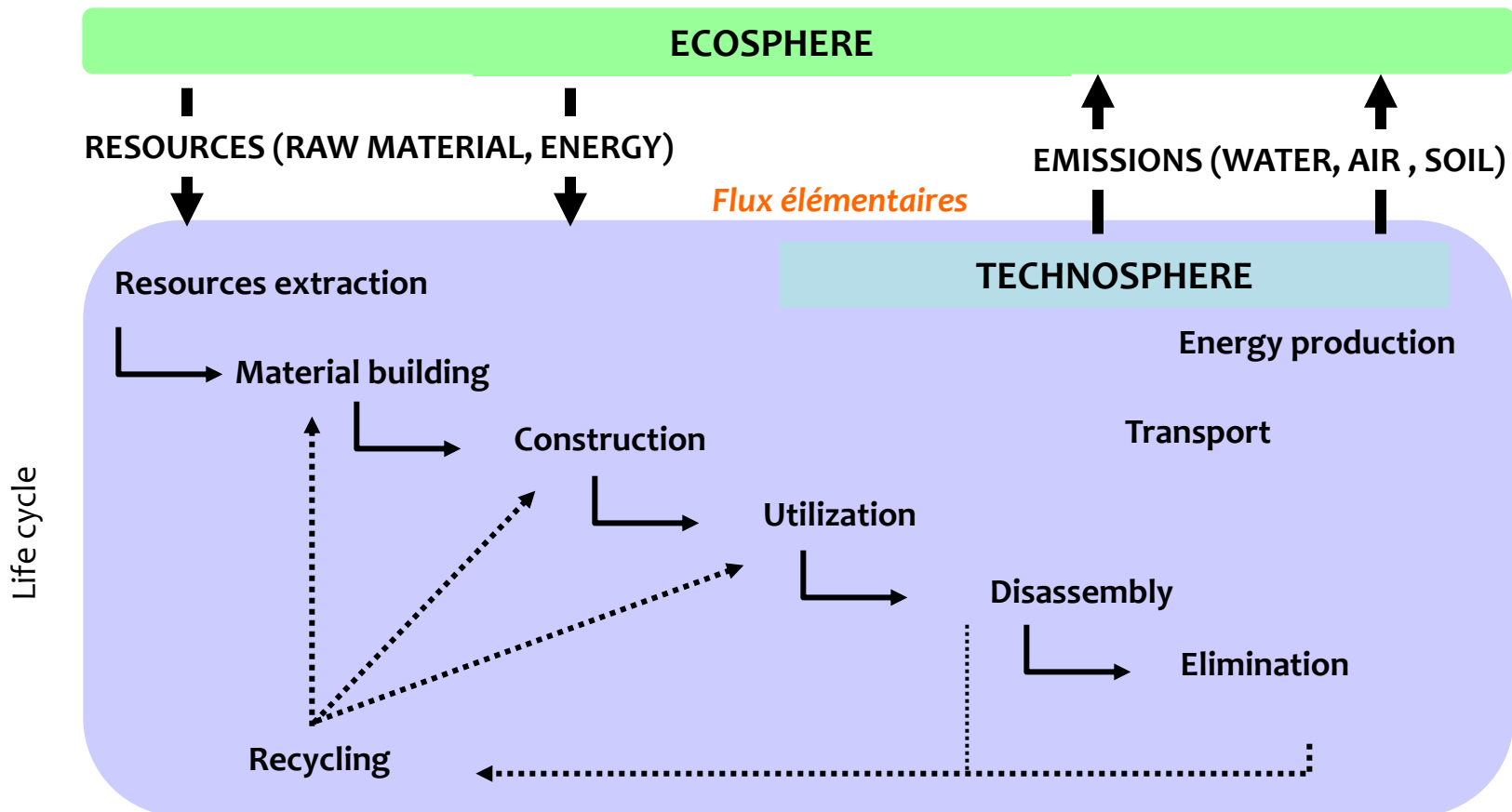
Stakeholder preferences and needs

Multi-criteria flexible querying

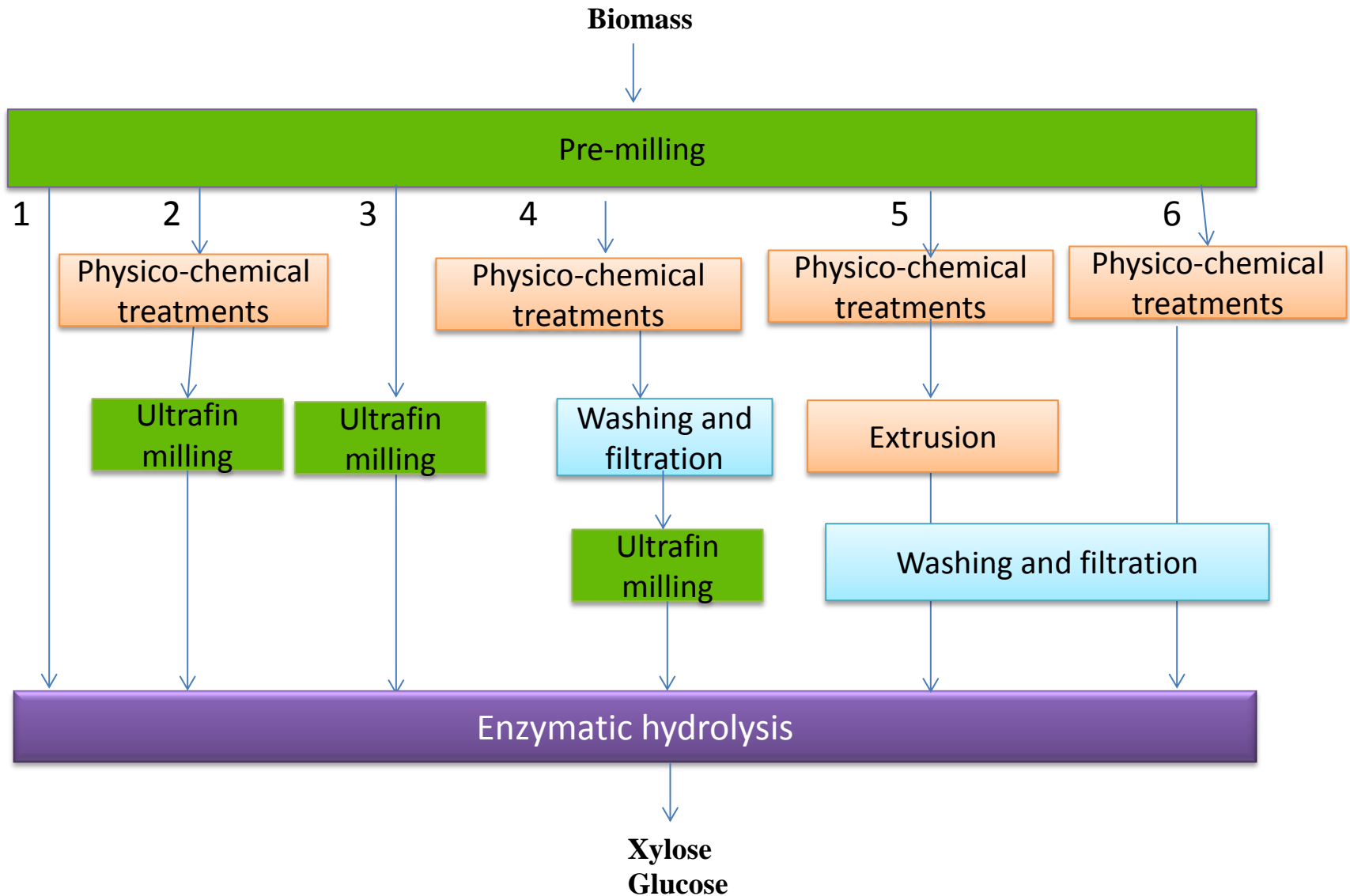
Packaging database

Ranked list of most relevant packagings

❖ **Life cycle analysis (LCA)** permits to estimate environmental impacts using a complete inventory of matter flow, energy, and effluents generated by the production process.

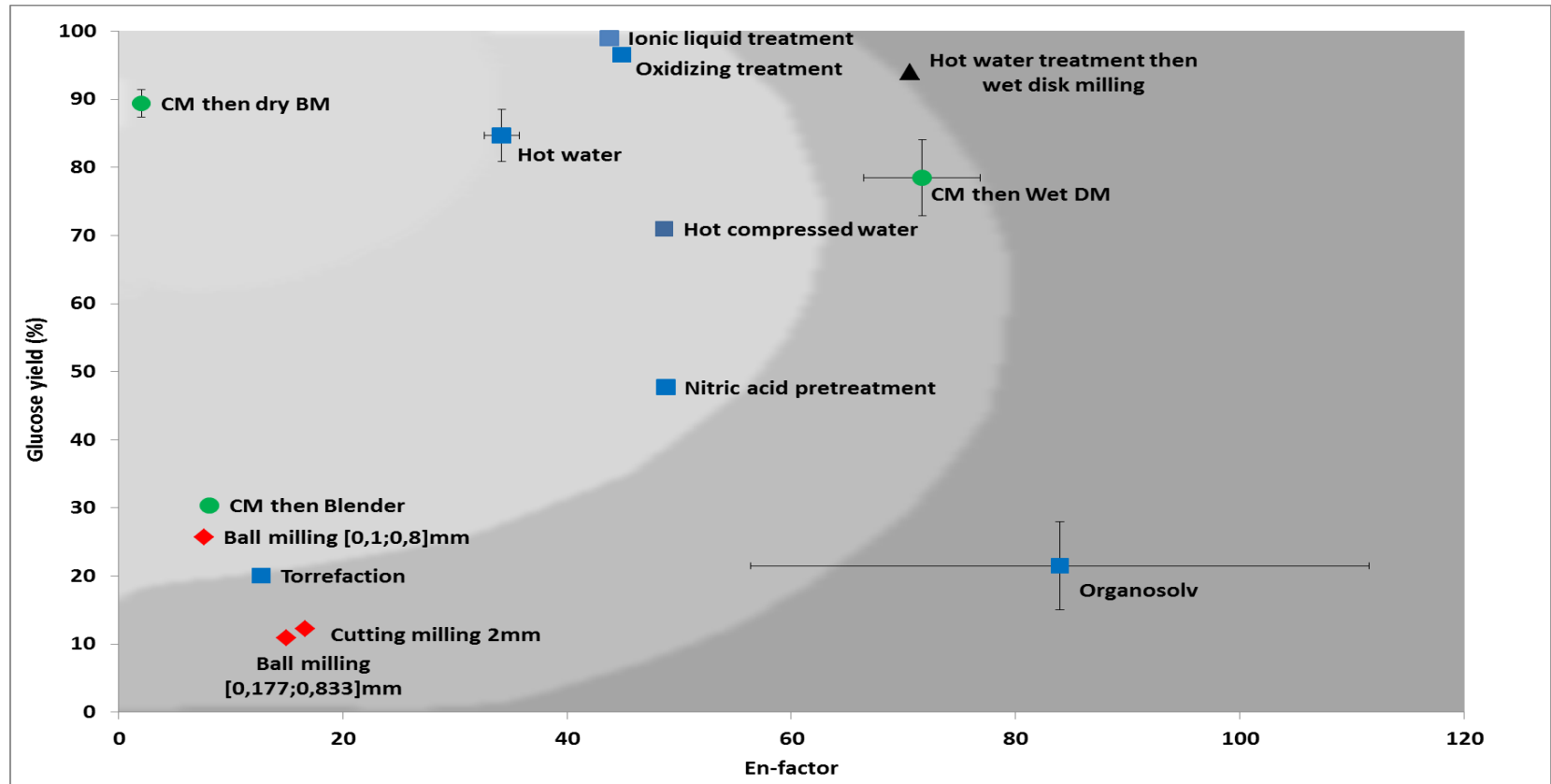


# Pre-treatment eco-design





# Pre-treatment comparison for rice straw



■ PM-PC-PS    
 ◆ PM    
 ● PM-UFM    
 ▲ PM-PC-UFM-PS

Projet IC2ACV – 24 septembre 2014



# Heterogeneous data capitalisation guided by an ontology

(Touhami et al. 2011, Buche et al. 2011, Berrahou et al. 2013, Touhami et al. 2013, Buche et al. 2013a, Destercke et al. 2013, Buche et al. 2013b, Buche et al. 2014 submitted)



Table 1: Permeabilities of MFC films and literature values for films of synthetic polymers and cellophane

| <u>Sample</u> | <u>Grammage</u><br>(g/m <sup>2</sup> ) | <u>Thickness</u><br>( $\mu$ m) | <u>Air permeability</u><br>(nm/Pa s) | <u>Oxygen permeability</u><br>in the material<br>(ml m <sup>-2</sup> day <sup>-1</sup> ) |
|---------------|--|--------------------------------|--------------------------------------|--|
| MFC film A    | 17 $\pm$ 1                             | 21 $\pm$ 1                     | 13 $\pm$ 2                           | 17.0, 18.5   |
| EVOH          | –                                      | 25                             | –                                    | 3–5  |
| Cellophane    | –                                      | 21                             | –                                    | 3  |

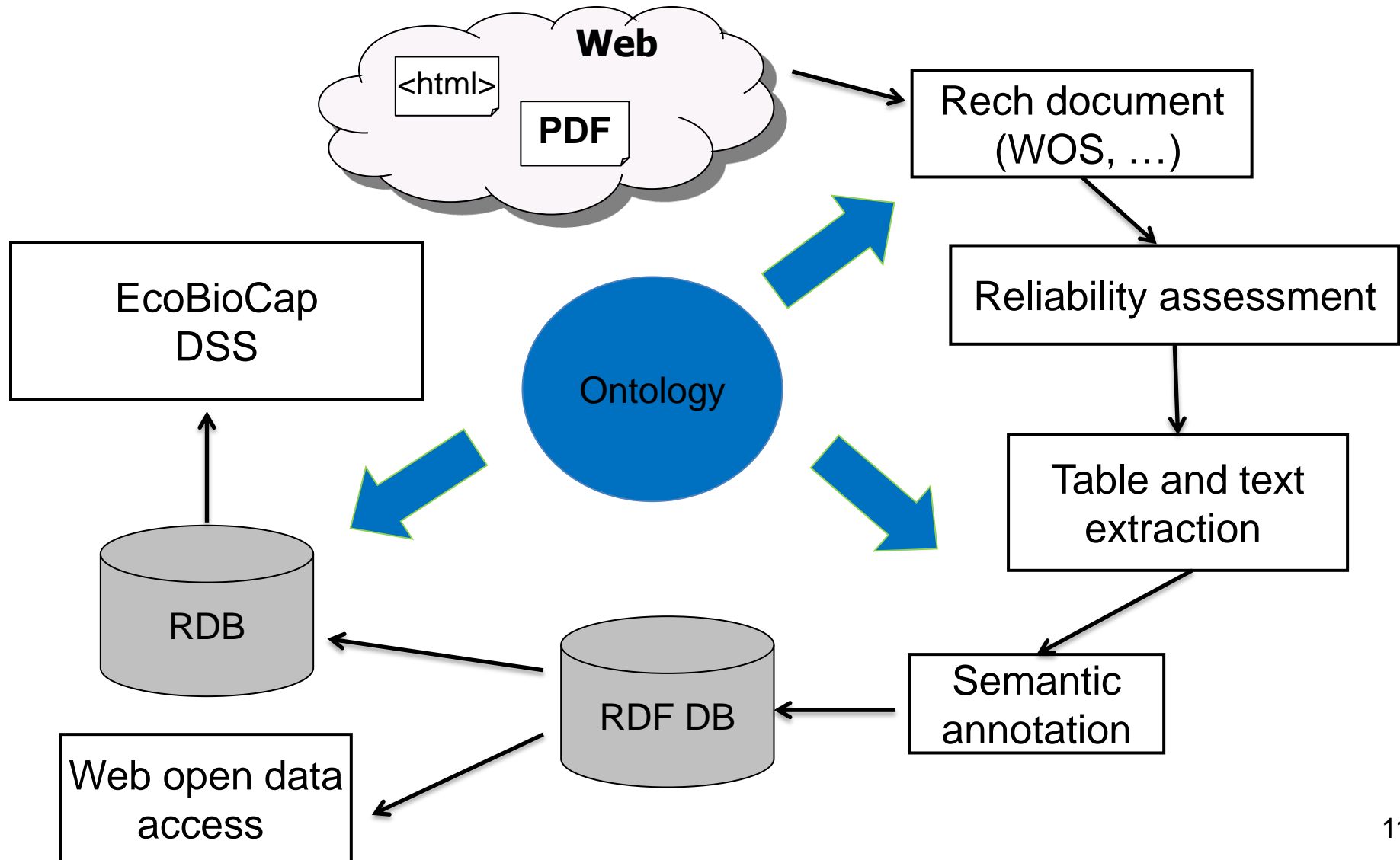
Symbolic concept  
Ethylene Vinyl Alcohol

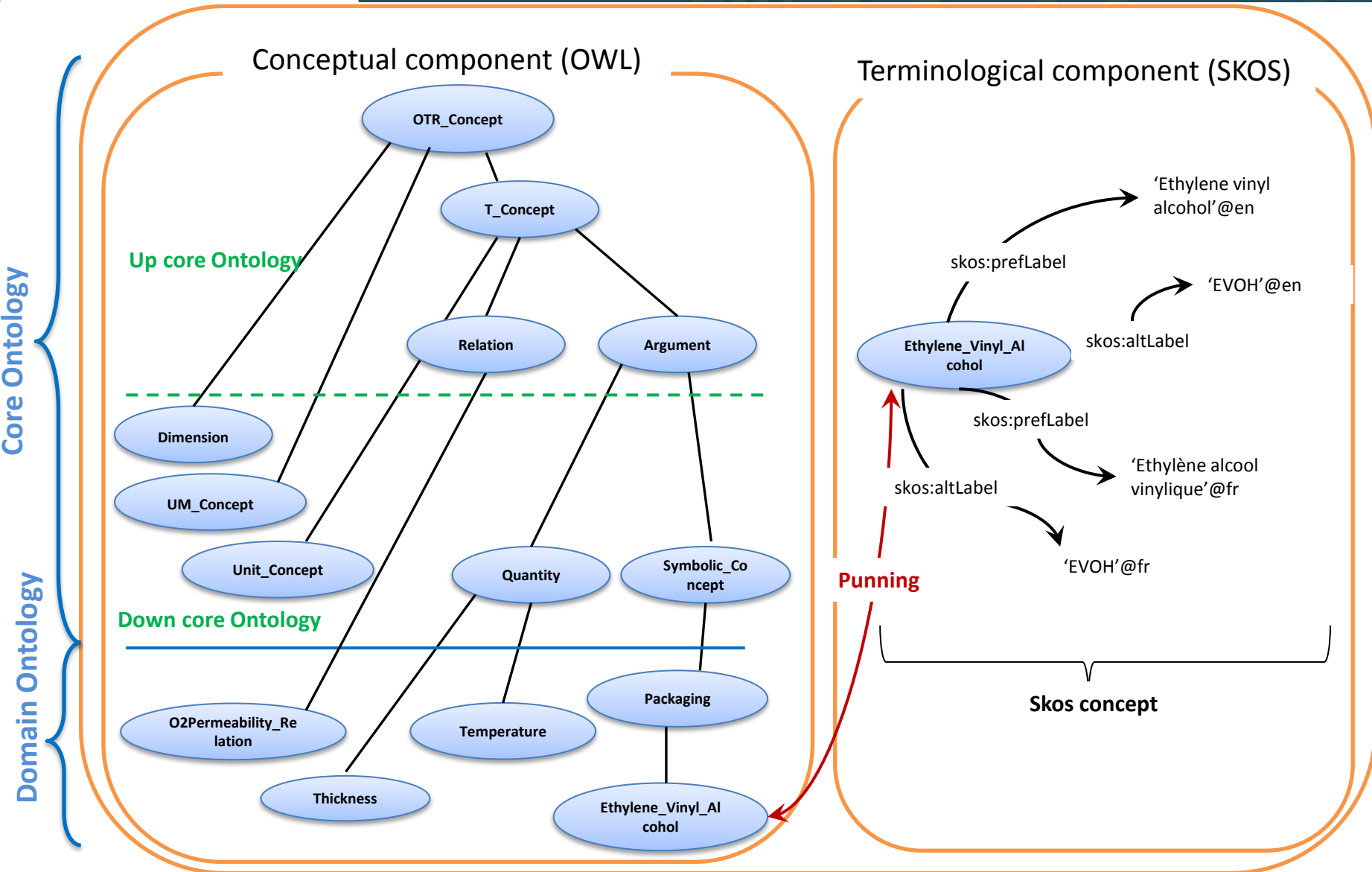
Symbolic concept  
Packaging

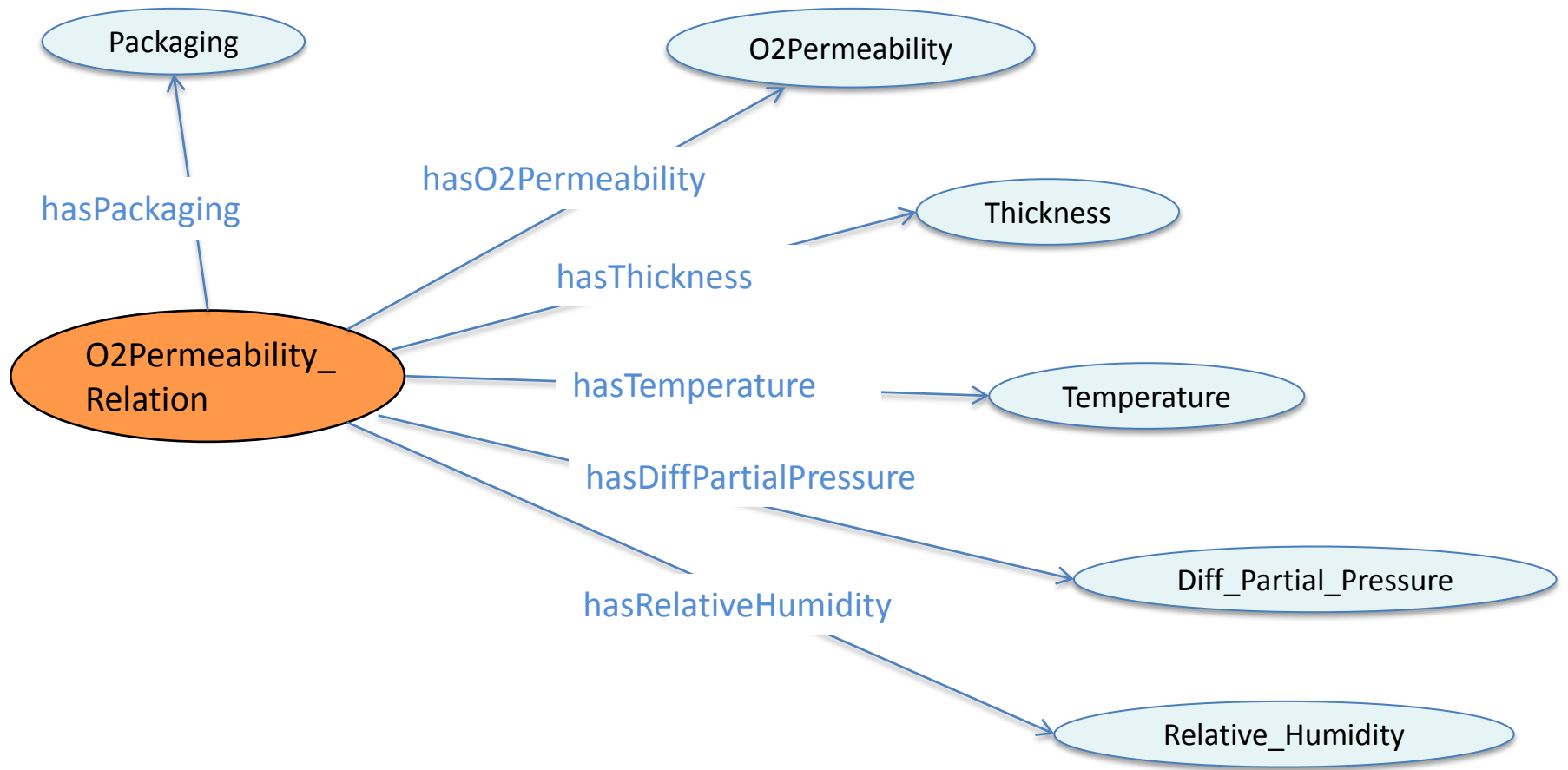
Quantity Thickness

Quantity O2Permeability

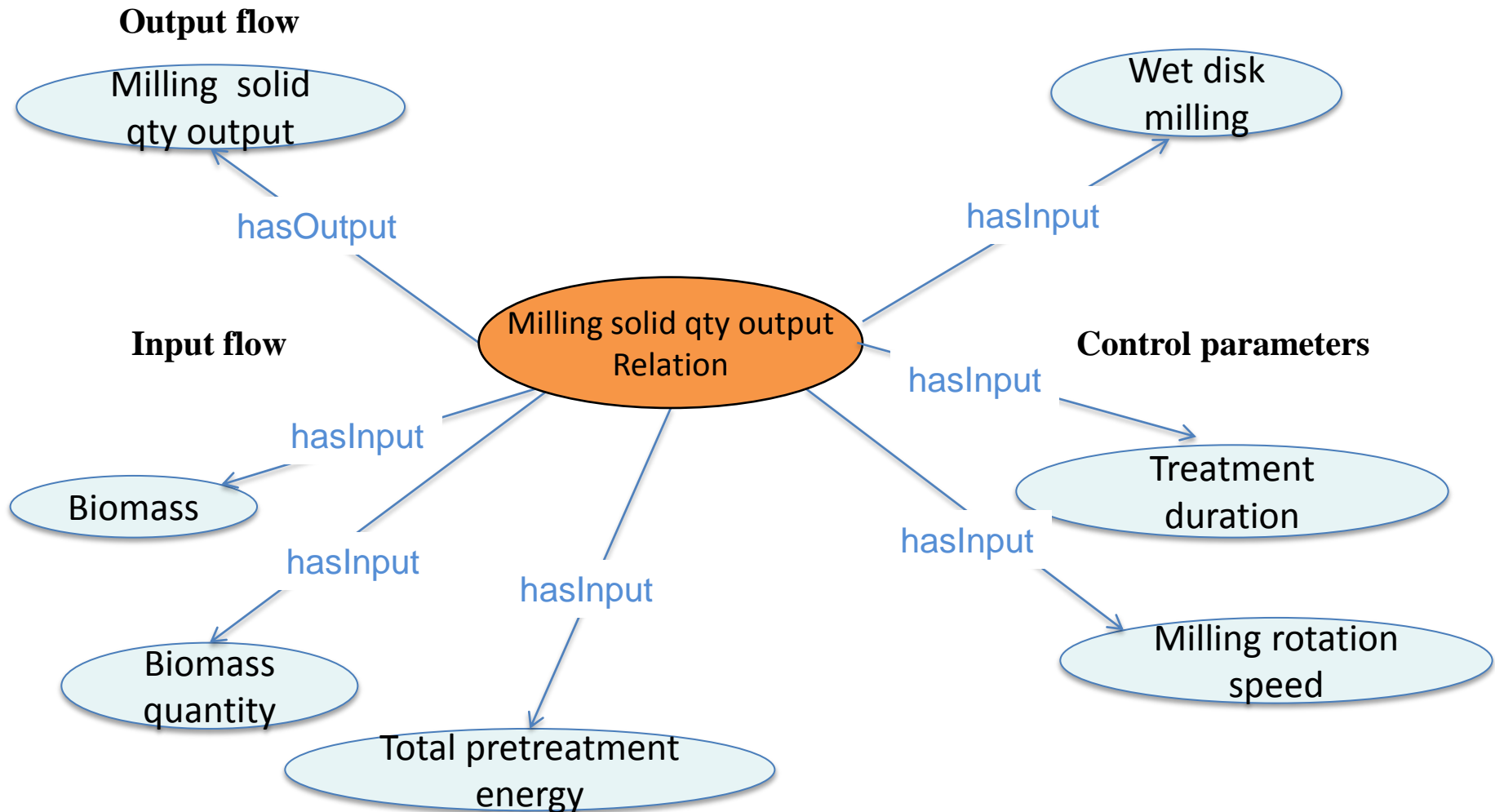
O2Permeability\_Relation





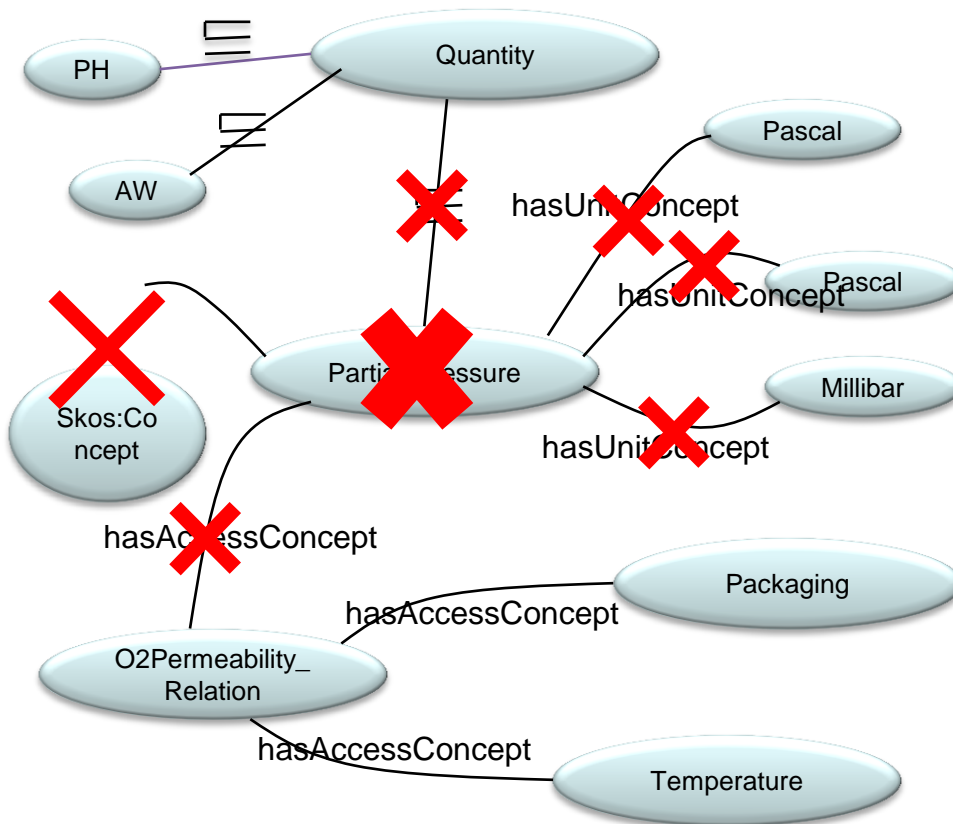


## A relation concept models a unit operation





Exemple : Supprimer la quantité partial\_pressure :



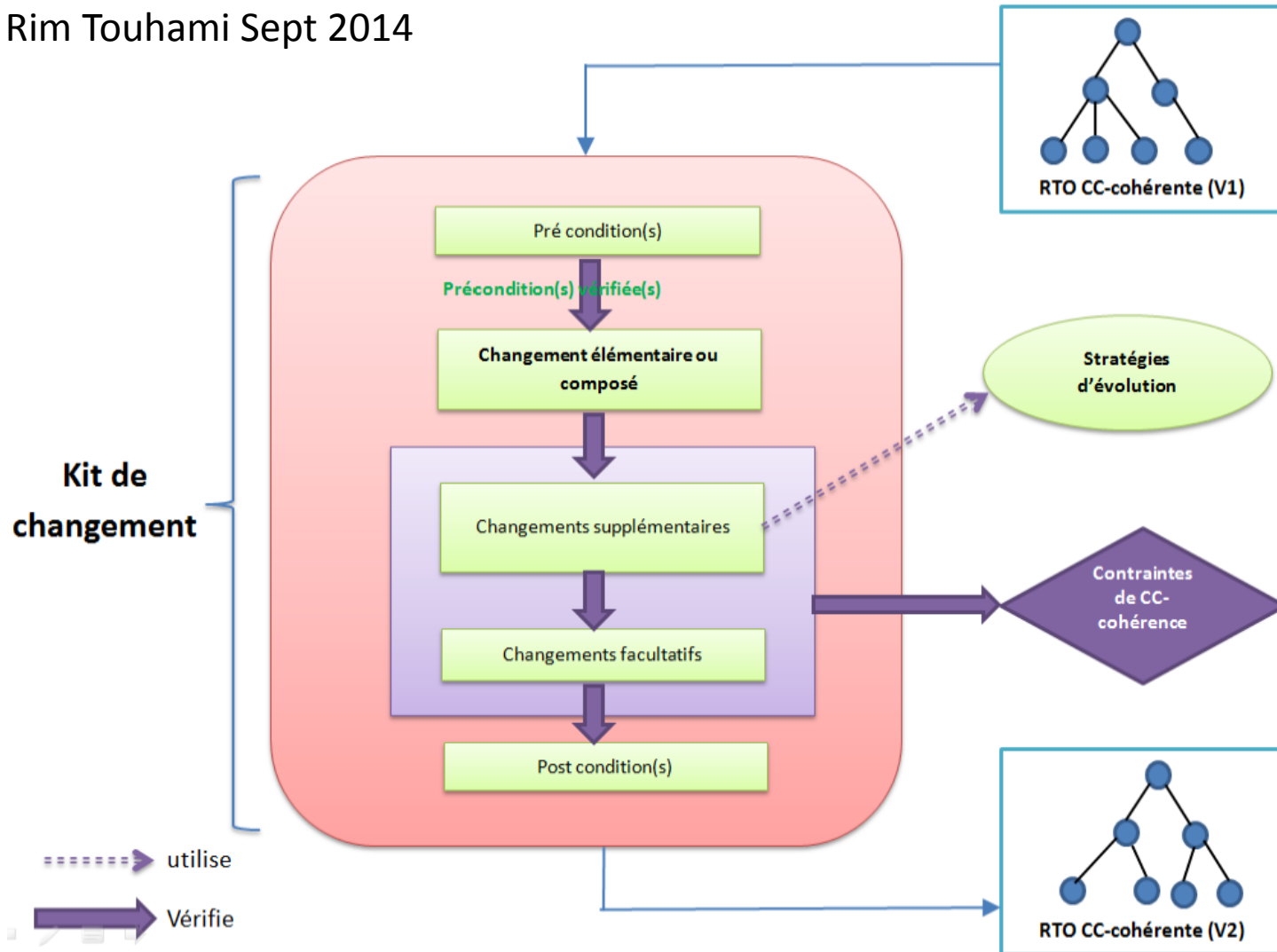
- Supprimer le lien d'hierarchie entre le concept générique Quantity et le concept partial\_pressure.
- Supprimer les liens avec les propriétés ayant partial\_pressure comme domaine.
- Supprimer les liens avec les propriétés ayant partial\_pressure comme co-domaine
- Supprimer la terminologie associée à partial\_pressure.

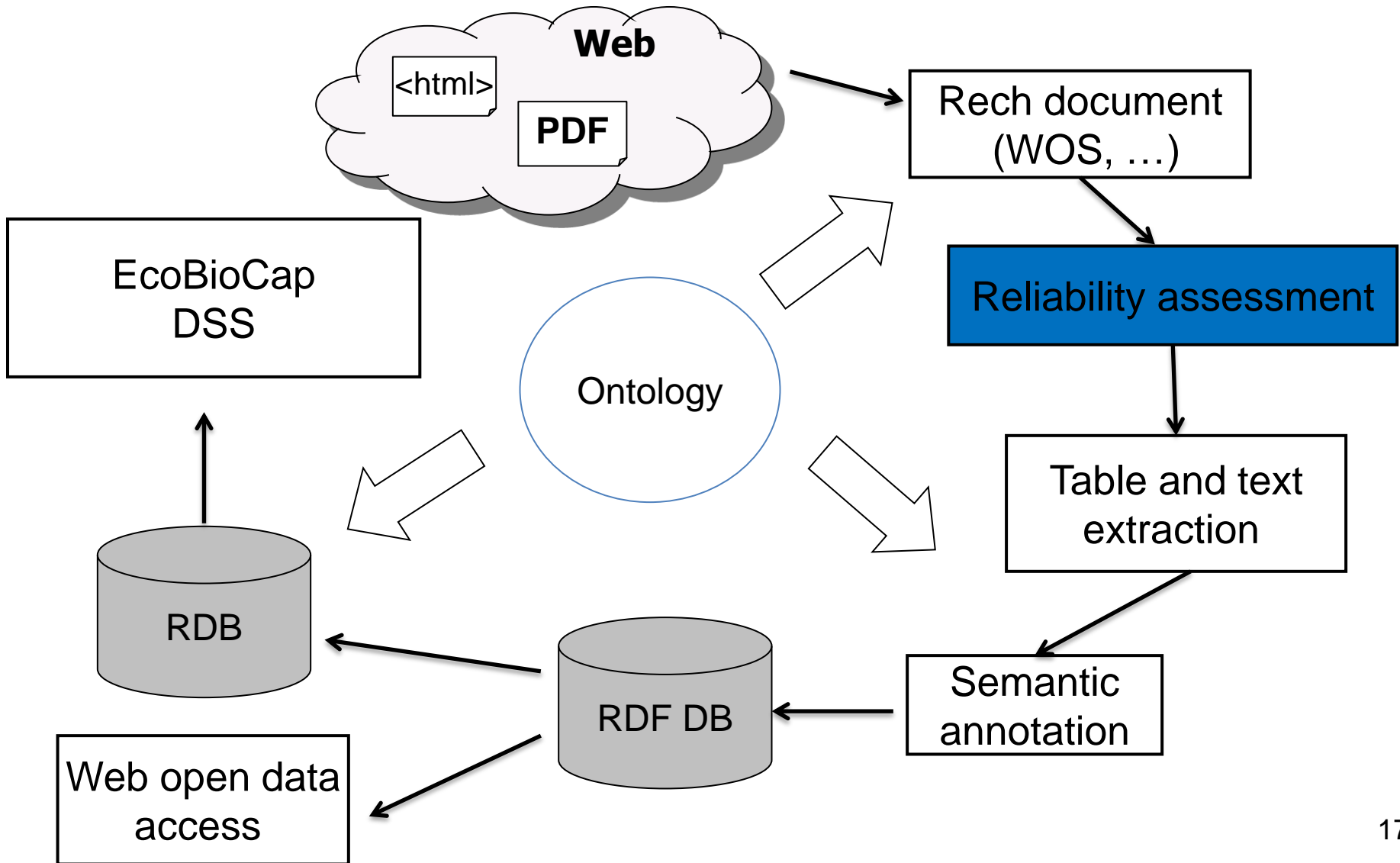
...





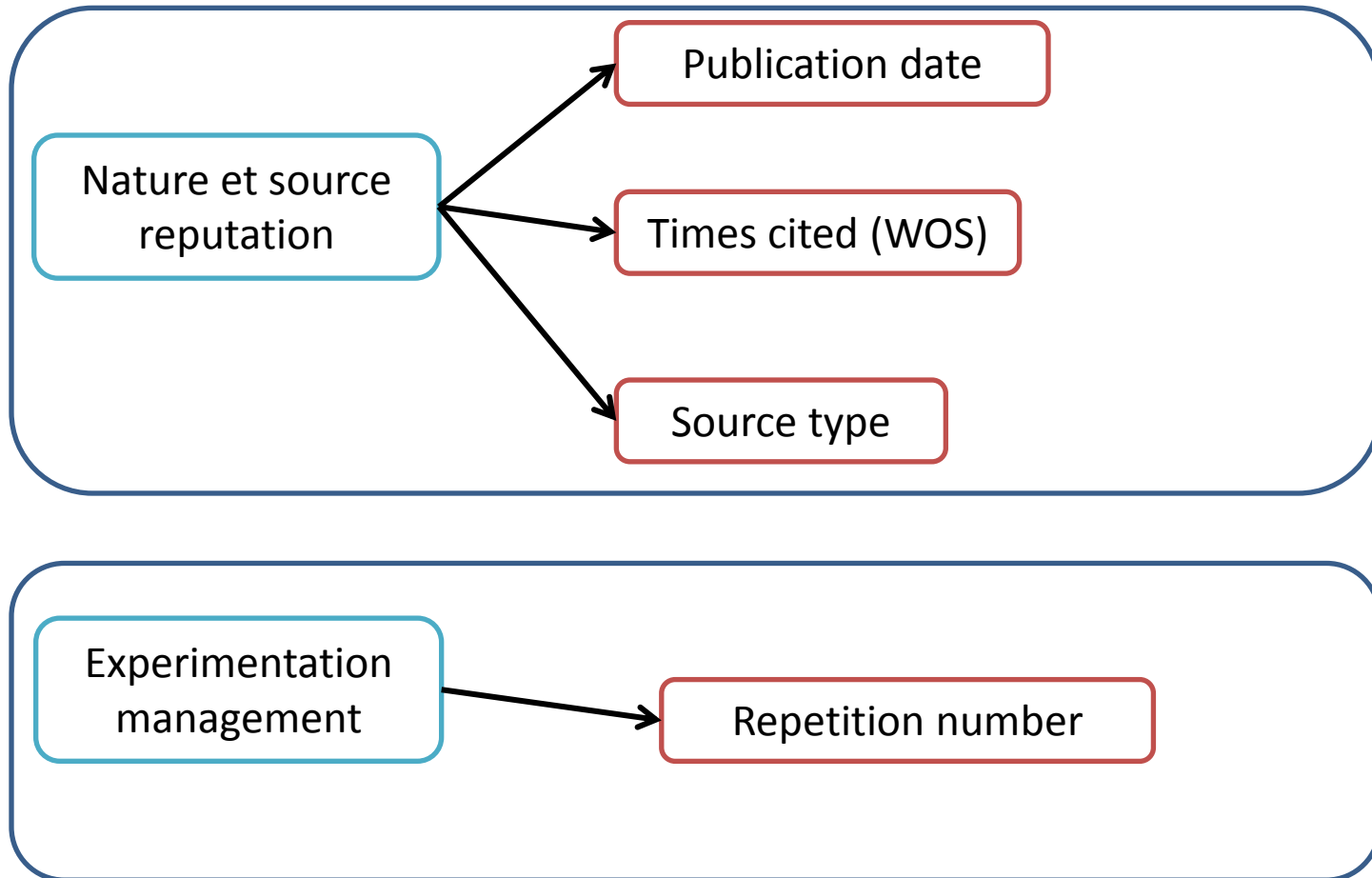
Thèse Rim Touhami Sept 2014







❖ 2 categories of meta data :





|   | unknown | not at all reliable | not at all or hardly | hardly reliable | hardly or average | average reliable | average or reliable | reliable | reliable or very | very reliable |
|---|---------|---------------------|----------------------|-----------------|-------------------|------------------|---------------------|----------|------------------|---------------|
| <b>repetition</b>   |         |                     |                      |                 |                   |                  |                     |          |                  |               |
| > No  |         | :                   |                      |                 |                   |                  |                     |          |                  |               |
| > Yes   |         |                     |                      |                 |                   |                  |                     |          |                  | ++            |
| <b>number of repetitions</b>                              |         |                     |                      |                 |                   |                  |                     |          |                  |               |
| > no repetition   |         | ::                  |                      |                 |                   |                  |                     |          |                  |               |
| > once  |         | ::                  |                      |                 |                   |                  |                     |          |                  |               |
| > twice   |         |                     |                      |                 |                   | -+               |                     |          |                  |               |
| > 3 times   |         |                     |                      |                 |                   |                  |                     | +        |                  |               |
| > more than 3 times                                       |         |                     |                      |                 |                   |                  |                     |          |                  | ++            |
| <b>age and citation number</b>                            |         |                     |                      |                 |                   |                  |                     |          |                  |               |
| > between 3 and 8 years old & less than 10 citations      |         |                     | [--, -]              |                 |                   |                  |                     |          |                  |               |
| > between 3 and 8 years old & between 10 and 20 citations |         |                     |                      |                 | [-, -+]           |                  |                     |          |                  |               |
| > between 3 and 8 years old & between 20 and 40 citations |         |                     |                      |                 |                   |                  | [-+, +]             |          |                  |               |

@Web graphical user interface



- MapOptropic
- MapOpt\_demo
- PackPermeability
  - An Overview of Pol**
  - Application of biopl
  - BRODART technica
  - Barrier and surface
  - Barrier properties o
  - Characterization of
  - Characterization of
  - Combined effects o
  - Danapak flexibles t
  - Effect of plasticizers
  - Evaluation of a Bio-
  - Fully Aliphatic Copo
  - Gas transfer proper
  - Layer-by-layer asse
  - Mechanical propert
  - Metabolix Mvera da
  - Morphology and Ba
  - Nanocomposites fo
  - Oxygen Permeabilit
  - Oxygen barrier of n

Citation Number : more than 40

Age : more than 8 years old

**Criterion age and top citation**


Age : more than 8 years old

Top Citation : top 0.10%

**Criterion source type**

Source Type : journal article

## Reliability evaluation's document information

**Reliability results** 

Low expectation : 4.94 ; High expectation : 5.0





Known criteria values rate : 80 %

**Last evaluation date** : 2014-09-29

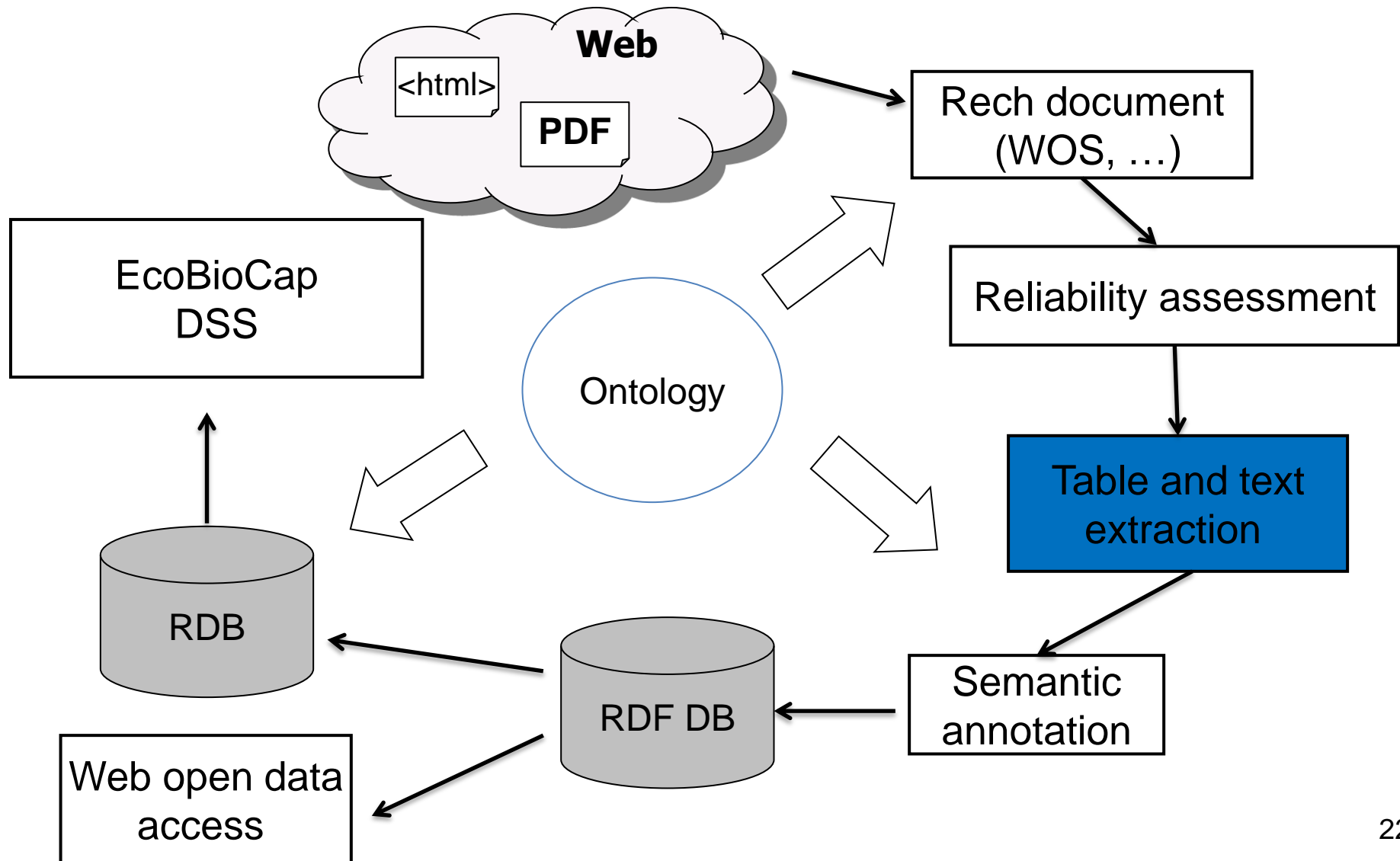
@Web graphical user interface



- [-] PackPermeability
  - [+] An Overview of Po
  - [x] Application of biop
  - [x] BRODART technic
  - [+] Barrier and surface
  - [+] Barrier properties c
  - [+] Characterization of
  - [x] Characterization of
  - [+] Combined effects c
  - [x] Danapak flexibles
  - [+] Effect of plasticizer
  - [x] Evaluation of a Bio
  - [+] Fully Aliphatic Cop
  - [+] Gas transfer prope
  - [x] Layer-by-layer ass
  - [+] Mechanical proper
  - [x] Metabolix Mvera d
  - [+] Morphology and Bi
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  - [x] Oxygen Permeabil
  - [x] Oxygen barrier of r
  - [x] Poly(lactic acid) Ne
  - [x] Polyimide Silica Co
  - [+] Prediction of water
  - [x] PropaFresh P2G
  - [+] Quince seed mucil
  - [+] Soluble soybean p
  - [+] Soy protein e Poly
  - [+] Structure property
  - [+] Suitability of novel
  - [+] Water barrier prop

| Classes             |   | Number of publications | Reliability Interval |
|---------------------|---|------------------------|----------------------|
| Very reliable       |  | 14                     | [ 4,97 ; 5 ]         |
| Reliable            |  | 3                      | [ 3,2 ; 4,85 ]       |
| In conflict         |  | 9                      | [ 1,01 ; 4,93 ]      |
| Not at all reliable |  | 4                      | [ 1,02 ; 1,33 ]      |

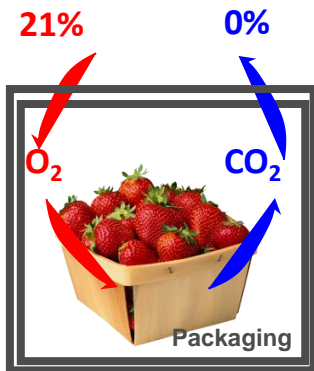
- Very reliable: peer-reviewed articles , with repetitions, high reputation
- Reliable: peer-reviewed articles, with repetitions, medium reputation
- In conflict: peer-reviewed articles but no repetition
- Not at all reliable: technical sheets without external review and no repetition







## Extracting experimental data



Experiments

The oxygen permeability was measured according to the ASTM standard D3985 (23 °C, 0% RH on the top side, 50% RH on the bottom side). The MFC films were mounted in a cell where 100% O<sub>2</sub> was flushed on the top side and 100% N<sub>2</sub> on the bottom side. The amount of O<sub>2</sub> transferred through the films was assessed by a Mocon Coulox oxygen sensor in the N<sub>2</sub> gas flow. Two replicates were measured for each sample.

### Results and Discussion

#### Parametrization

To perform the program, the parameters involved in equations must be estimated.

The permeability of the LDPE film was estimated independently by the cell permeability method. At 100% relative humidity and 20 °C, O<sub>2</sub> and CO<sub>2</sub> permeability were respectively 1078 and 4134 amol × m<sup>-2</sup> × s<sup>-1</sup> × Pa<sup>-1</sup>. These values did not change significantly when the relative humidity decreased (data not shown) and were in close agreement with the literature data for the same material (Pauly 1989).

To design an oxygen-absorber equation, typical experimental data for ATCO® LH100 compared with time are presented in Figure 1. The following absorption kinetic model was fitted to the experimental data and was a typical saturation exponential curve. The following mathematical model was then developed to express the number of oxygen moles absorbed ("N<sub>O<sub>2</sub></sub>") compared with time:

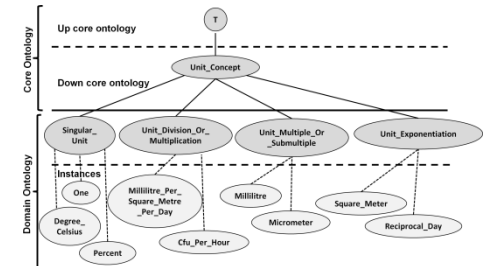
#### Materials and Methods

##### Materials

Tomatoes ('Grace') were shipped by the Centre technique inter-professionnel des fruits et légumes (CTIFL) of Saint-Remy de Provence (France) to the laboratory within 24 hours after harvesting. They were obtained from a local producer in Arles, France. They were kept at 20 °C under ambient air for 12 h before the experiments began.

Low density polyethylene film of 50 µm thickness was used (LDPE: BBA Emballage - Manu Pack, St-Jean de Vedas, France). Oxygen absorbers, type ATCO® LH100, were supplied by Stan-

Published experimental data in scientific documents



Enriching an Ontological and Terminological Resource (OTR)

## Quantitative data

{(LDPE, Packaging: (Low Density Polyethylene)),  
(50 µm, Thickness: (value: 50, unit concept: Micrometer)),  
( 1078 amol x m-1 x s-1 x Pa-1, O2Permeability : (value: 1078, unit concept: Attomole per meter per second per pascal))}

Localisation of relevant information (packaging characteristics)





Reduction of the search space in the text and enrichment of the termino-ontological resource by adding units of measure

## Motivation

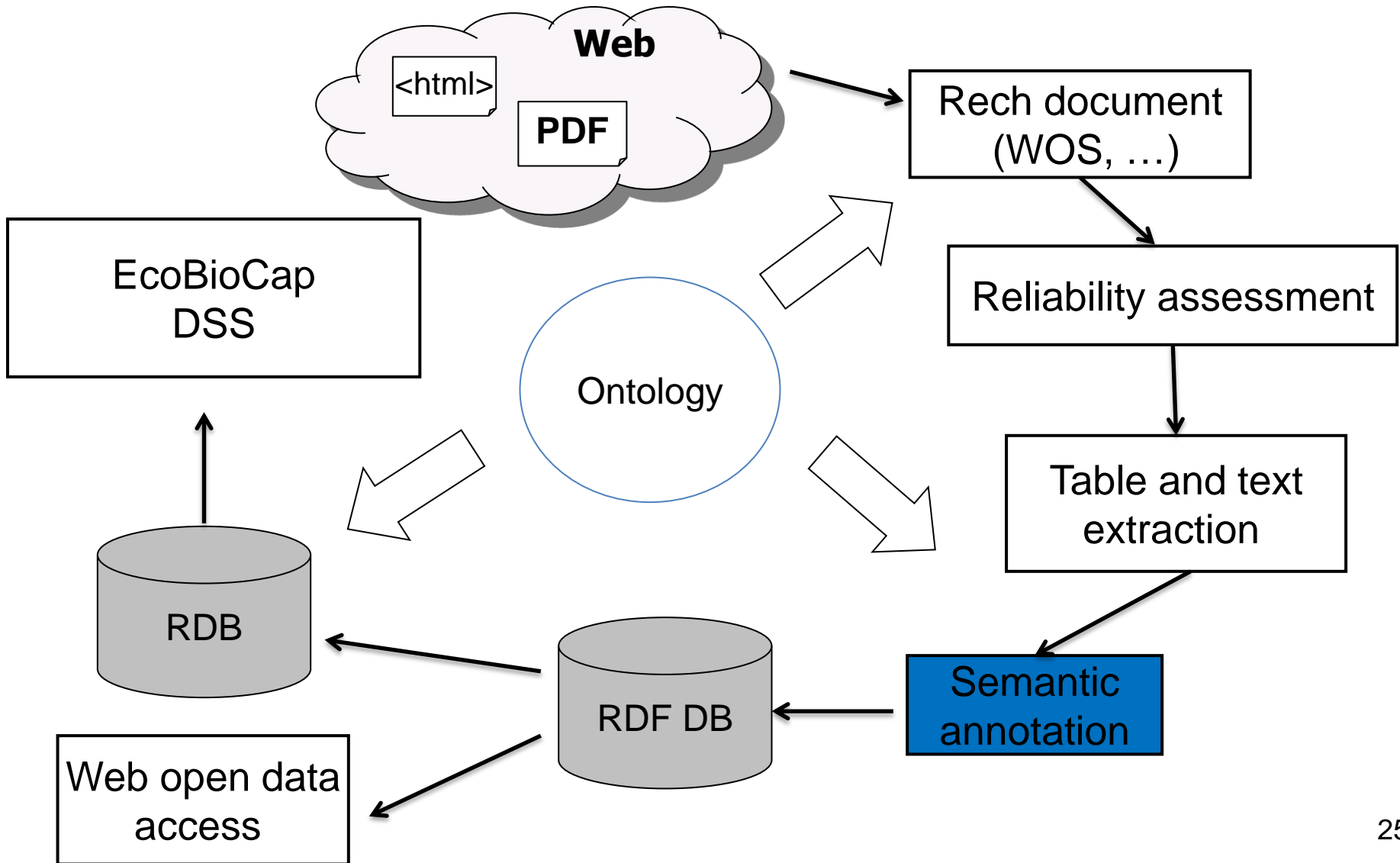
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### Automatic extraction from the text of quantitative data

- Water Vapor Permeability (WVP) of  $1.81 \times 10^{-9} \text{ g m}^{-1} \text{ s}^{-1} \text{ Pa}^{-1}$
- O<sub>2</sub> permeability increasing from 7.12 to  $7.68 \times 10^{-15} \text{ g} \cdot (\text{Pa s m})^{-1}$

## Scientific locks

- 
- ❖ Locate relevant information in the text
  - ❖ Identify and extract units of measure taking into account their specific syntactical rules





|  |                    |
|--|--------------------|
| <b>▼ PrefLabel</b>   | <b>▼ Hierarchy</b> |
| Relation de perméabilité au dioxyde de carbone (fr)<br>CO2 Permeability_Relation (en)  |                    |
| <b>▶ AltLabel</b>  |                    |
| <b>▼ ScopeNote</b>   |                    |
| <p>- In an annotated table, when both O2 and CO2 permeabilities are in the same table but measured at different temperature, enter information for O2 on a row and for CO2 on the next row. Empty cellars are authorized in the table (en)</p> <p>- About partial pressure, look for missing information in the material and methods. From the description of the methodology of O2/CO2 permeability measurements or from the name of the standard use (ASTM, DIN, etc ...), check the difference if partial pressure applied to the film and add this information (min – max span) in the table (en)</p> <p>- For relative humidity, if not available publication could be nevertheless kept with missing RH (en)</p> <p>- For relative humidity, check in the material and methods the value of RH set up for the measurement and add this information in the table (could be not directly written in the paper but may be known from the name of the standard used) (en)</p> <p>- In a review paper, if the unit of measure associated with the O2/CO2 permeability value includes both pressure and thickness dimensions (by example mol/m/s/Pa), the data may be entered even if pressure and thickness data are lacking (en)</p> <p>- About partial pressure, if information is not available and if the unit associated with the CO2 permeability measure does not include the pressure, discard the publication because data could be not further usable without this data. (en)</p> |                    |
| <b>▼ Relation</b>  |                    |
| <b>Result :</b> <ul style="list-style-type: none"> <li>• CO2 Permeability</li> </ul>   |                    |
| <b>Access :</b> <ul style="list-style-type: none"> <li>• Partial pressure difference</li> <li>• Packaging</li> <li>• Relative Humidity</li> <li>• Temperature</li> <li>• Thickness</li> </ul>  |                    |

@Web graphical user interface



## Manual Annotation of Oxygen Permeability of the Various Samples at 0% RH and at 80% RH and Estimated Diffusion and Solubility...

### Original table

TableIII. Oxygen Permeability of the Various Samples at 0% RH and at 80% RH and Estimated Diffusion and Solubility Coefficients at 80% RH for the Blends

| Sample                   | PO <sub>2</sub> (m <sup>3</sup> m/m <sup>2</sup> s Pa) 24°C, 0% RH | PO <sub>2</sub> (m <sup>3</sup> m/m <sup>2</sup> s Pa) 80% RH | DO <sub>2</sub> (m <sup>2</sup> /s) 80% RH | SO <sub>2</sub> (m <sup>3</sup> /m <sup>3</sup> Pa) 80% RH |
|--------------------------|--|---|--|--|
| PHB-Blend                | <sup>a</sup> 4.2 ± 0.0005 e <sup>-19</sup>                         | <sup>a</sup> 5.2 ± 0.004 e <sup>-19</sup>                     | <sup>a</sup> 1.1 ± 0.01 e <sup>-12</sup>   | <sup>a</sup> 4.7 ± 0.05 e <sup>-7</sup>                    |
| (14.6 e <sup>-19</sup> ) |  |   |  |  |
| (4.0 e <sup>-19</sup> )  |  |   |  |  |
| 1%NanoterPHB-Blend       | <sup>b</sup> 3.8 ± 0.3 e <sup>-19</sup>                            | <sup>b</sup> 3.9 ± 0.1 e <sup>-19</sup>                       | <sup>b</sup> 1.0 ± 0.02 e <sup>-12</sup>   | <sup>b</sup> 3.9 ± 0.2 e <sup>-7</sup>                     |

### Annotated table

| n° | Thickness Unit : mm     | Temperature Unit : °C | Relative_Humidity Unit : % | Packaging   | Partial pressure difference Unit : Pa | O2 Permeability Unit : m <sup>3</sup> .m/(m <sup>2</sup> .s.Pa) |
|----|-------------------------|-----------------------|----------------------------|---|---------------------------------------|---|
| 1  | [ 1.000e-1 ; 9.000e-1 ] | 2.400e1               | 0.000e0                    | Polyhydroxybutyrate/Polycaprolactones             | [ 0.000e0 ; 1.013e5 ]                 | [ 4.199e-19 ; 4.200e-19 ]                                       |
| 2  | [ 1.000e-1 ; 9.000e-1 ] | 2.400e1               | 0.000e0                    | (1%Nanoter) Polyhydroxybutyrate/Polycaprolactones | [ 0.000e0 ; 1.013e5 ]                 | [ 3.500e-19 ; 4.100e-19 ]                                       |
| 3  | [ 1.000e-1 ; 9.000e-1 ] | 2.400e1               | 0.000e0                    | (4%Nanoter) Polyhydroxybutyrate/Polycaprolactones | [ 0.000e0 ; 1.013e5 ]                 | [ 2.100e-19 ; 2.700e-19 ]                                       |
| 4  | [ 1.000e-1 ; 9.000e-1 ] | 2.400e1               | 0.000e0                    | Polyhydroxybutyrate                               | [ 0.000e0 ; 1.013e5 ]                 | [ 2.298e-19 ; 2.302e-19 ]                                       |
| 5  | [ 1.000e-1 ; 9.000e-1 ] | 2.400e1               | 0.000e0                    | (4%Nanoter) Polyhydroxybutyrate                   | [ 0.000e0 ; 1.013e5 ]                 | [ 1.500e-19 ; 2.100e-19 ]                                       |
| 6  | [ 1.000e-1 ; 9.000e-1 ] | 2.400e1               | 0.000e0                    | Polycaprolactones                                 | [ 0.000e0 ; 1.013e5 ]                 | 5.800e-18   |
| 7  | [ 1.000e-1 ; 9.000e-1 ] | 2.400e1               | 0.000e0                    | Polyethylen Terephthalate                         | [ 0.000e0 ; 1.013e5 ]                 | 3.300e-19   |
| 8  | [ 1.000e-1 ; 9.000e-1 ] | 2.400e1               | 8.000e1                    | Polyhydroxybutyrate/Polycaprolactones             | [ 0.000e0 ; 1.013e5 ]                 | [ 5.196e-19 ; 5.204e-19 ]                                       |

# @Web graphical user interface



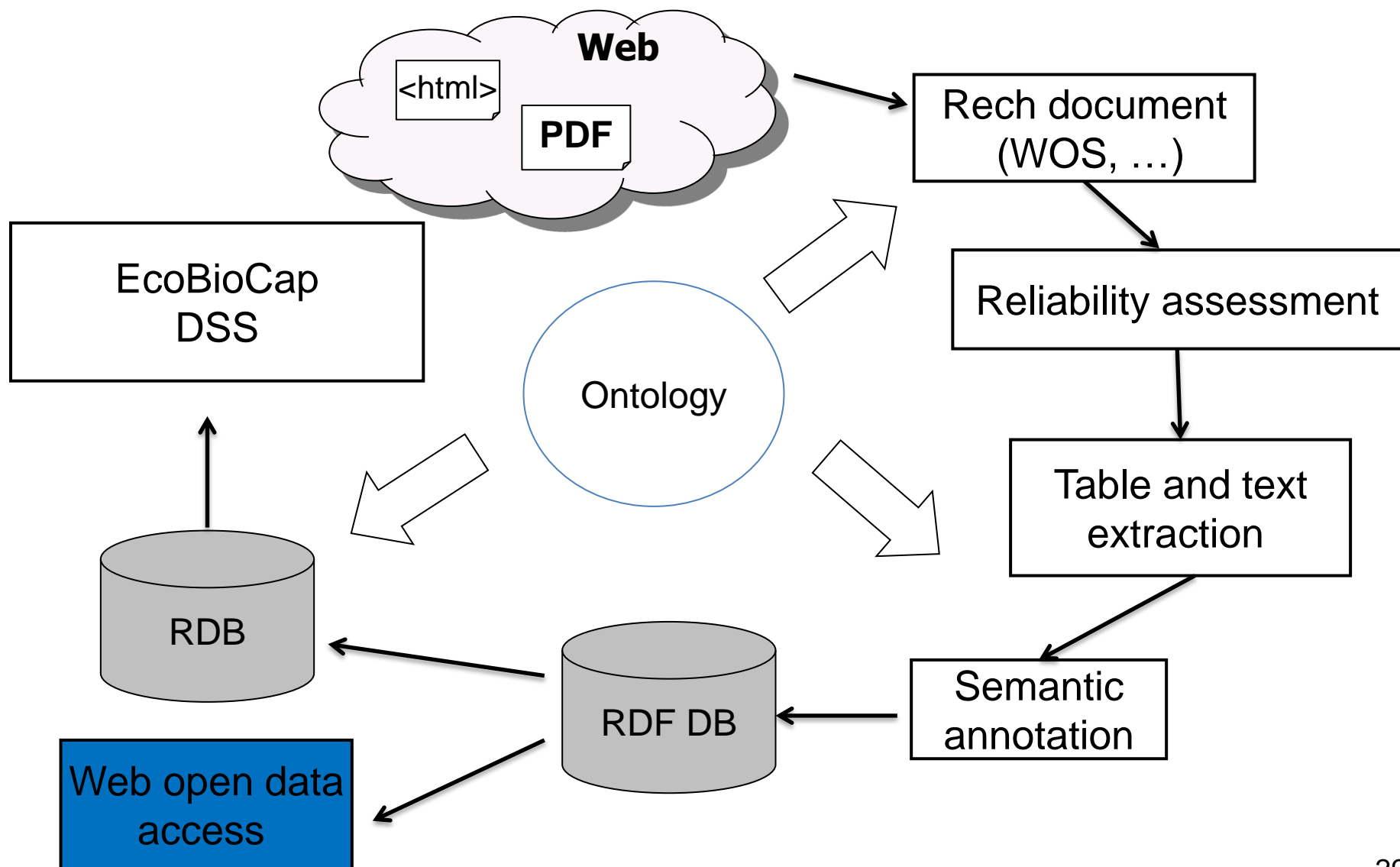
Manual Annotation of Comparison of sugar yields, crystallinity, and energy consumption between three pretreatments in various...

Original table

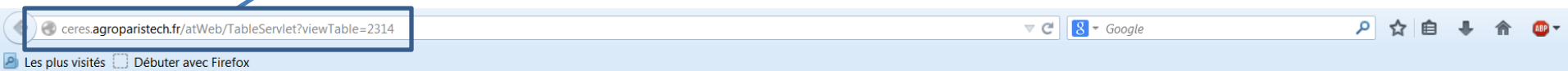
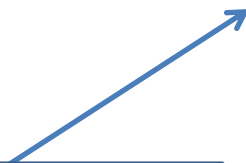
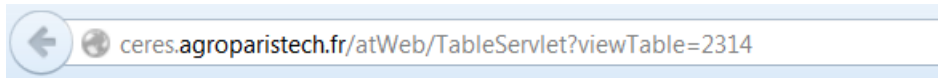
| Sample                | Sugar yields (%) |          | Crl (%)  |          | Energy consumption (MJ/kg rice straw) |     |  |
|-----------------------|------------------|----------|----------|----------|---------------------------------------|-----|--|
|                       | Xyl              | Ara      | Total    |          |                                       |     |  |
| CM                    | 23.4±2.3         | 18.7±2.7 | 29.7±1.4 | 22.5±1.3 | 51.9                                  | -   |  |
| DBM <sub>5 min</sub>  | 52.2±3.5         | 16.5±0.4 | 28.4±1.0 | 41.8±2.3 | 46.7                                  | 9.0 |  |
| DBM <sub>15 min</sub> | 66.0±0.5         | 28.0±0.3 | 34.3±0.4 | 54.5±0.4 | 35.0                                  | 27  |  |
| DBM <sub>30 min</sub> | 75.9±0.5         | 38.3±0.2 | 40.5±0.4 | 64.4±0.4 | 25.2                                  | 54  |  |
| DBM <sub>60 min</sub> | 89.4±2.0         | 54.3±1.3 | 48.9±1.0 | 78.2±1.7 | 13.3                                  | 108 |  |
| HCWT <sub>160</sub>   | 70.3±3.3         | 88.6±4.4 | 54.7±3.4 | 74.1±3.6 | 56.5                                  | 5.7 |  |

Annotated table

| n° | Output solid constituent size<br>Unit : mm | Treatment                      | Experience number<br>Unit : 1 | Process step number<br>Unit : 1 | Biomass    | Biomass quantity<br>Unit : g | Total pretreatment energy<br>Unit : MJ/kg | Water quantity<br>Unit : ml | Milling rotation speed<br>Unit : min-1 | Treatment duration<br>Unit : min | Output solid constituent quantity<br>Unit : g | Temperature<br>Unit : °C | Output liquor quantity<br>Unit : |
|----|--|--------------------------------|-------------------------------|---------------------------------|------------|------------------------------|---|-----------------------------|--|----------------------------------|---|--------------------------|----------------------------------|
| 1  | 2.000e+0                                   | Cutting milling                | 1.000e+0                      | 1.000e+0                        | Rice straw | 3.000e+1                     | [ -inf ; inf ]                            | 0.000e+0                    | [ -inf ; inf ]                         | [ -inf ; inf ]                   |   |                          |                                  |
| 2  |  | Drying                         | 1.000e+0                      | 2.000e+0                        | Rice straw | 3.000e+1                     | [ -inf ; inf ]                            |                             |  | [ -inf ; inf ]                   | 3.000e+1                                      | 6.000e+1                 |                                  |
| 3  |  | Hot water treatment            | 1.000e+0                      | 3.000e+0                        | Rice straw | 3.000e+1                     | 5.700e+0                                  | 3.000e+2                    |  | 3.000e+1                         | 3.000e+1                                      | 1.600e+2                 | 3.000                            |
| 4  |  | Enzymatic hydrolysis treatment | 1.000e+0                      | 4.000e+0                        | Rice straw | [ 4.000e-2 ; 6.000e-2 ]      |   |                             |  | 4.320e+3                         | [ 3.020e-2 ; 4.670e-2 ]                       | 4.500e+1                 |                                  |
| 5  | 2.000e+0                                   | Cutting milling                | 2.000e+0                      | 1.000e+0                        | Rice straw | 3.000e+1                     | [ -inf ; inf ]                            | 0.000e+0                    | [ -inf ; inf ]                         | [ -inf ; inf ]                   |   |                          |                                  |







CO<sub>2</sub> permeability  
([export](#))

| n° | CO <sub>2</sub> Permeability<br>Unit : kg.m.m-2.s-1.pa-1 | Partial pressure difference<br>Unit : atm | Packaging                           | Relative_Humidity<br>Unit : % | Temperature<br>Unit : °C | Thickness<br>Unit : µm |
|----|--|---|-------------------------------------|-------------------------------|--------------------------|------------------------|
| 1  | [ 2.720e+17 ; 2.820e+17 ]                                | [ -inf ; inf ]                            | poly(98% l-lactide)/Polylactic Acid | 0.000e+0                      | 2.500e+1                 | [ 0.000e+0 ; inf ]     |
| 2  | [ 1.930e+17 ; 2.050e+17 ]                                | [ -inf ; inf ]                            | poly(94% l-lactide)/Polylactic Acid | 0.000e+0                      | 2.500e+1                 | [ 0.000e+0 ; inf ]     |
| 3  | [ 3.070e+17 ; 3.170e+17 ]                                | [ -inf ; inf ]                            | poly(98% l-lactide)/Polylactic Acid | 0.000e+0                      | 3.000e+1                 | [ 0.000e+0 ; inf ]     |
| 4  | [ 2.230e+17 ; 2.350e+17 ]                                | [ -inf ; inf ]                            | poly(94% l-lactide)/Polylactic Acid | 0.000e+0                      | 3.000e+1                 | [ 0.000e+0 ; inf ]     |
| 5  | [ 3.360e+17 ; 3.480e+17 ]                                | [ -inf ; inf ]                            | poly(98% l-lactide)/Polylactic Acid | 0.000e+0                      | 3.500e+1                 | [ 0.000e+0 ; inf ]     |
| 6  | [ 2.460e+17 ; 2.580e+17 ]                                | [ -inf ; inf ]                            | poly(94% l-lactide)/Polylactic Acid | 0.000e+0                      | 3.500e+1                 | [ 0.000e+0 ; inf ]     |
| 7  | [ 3.720e+17 ; 3.840e+17 ]                                | [ -inf ; inf ]                            | poly(98% l-lactide)/Polylactic Acid | 0.000e+0                      | 4.000e+1                 | [ 0.000e+0 ; inf ]     |
| 8  | [ 2.830e+17 ; 2.910e+17 ]                                | [ -inf ; inf ]                            | poly(94% l-lactide)/Polylactic Acid | 0.000e+0                      | 4.000e+1                 | [ 0.000e+0 ; inf ]     |
| 9  | [ 4.030e+17 ; 4.330e+17 ]                                | [ -inf ; inf ]                            | poly(98% l-lactide)/Polylactic Acid | 0.000e+0                      | 4.500e+1                 | [ 0.000e+0 ; inf ]     |
| 10 | [ 3.290e+17 ; 3.410e+17 ]                                | [ -inf ; inf ]                            | poly(94% l-lactide)/Polylactic Acid | 0.000e+0                      | 4.500e+1                 | [ 0.000e+0 ; inf ]     |



## Query Summary

| Query scope |  |
|-------------|--|
| Ontology    | IC2ACV   |
| Topics      | "Bioref-PM-PC-UFM", "Bioref-PM-PC-UFM-PS", "Bioref-PM-UFM", "Bioref-PM-PC-EX-PS", "Bioref-PM-PC-PS", "Bioref-PM" |
| Relation    | Biomass glucose composition relation   |

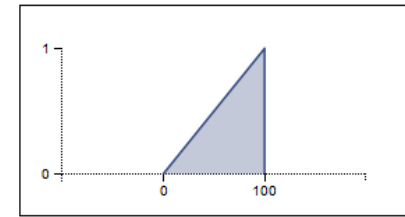
### Value domains wanted for attributes

- Mandatory**  
(1) Biomass : [ Grasses and energetic plants : 1 ]
- Desirable**  
(1) Glucose rate : [ 0 ; 100 ; 100 ; 100 ] - unit : Percent

### Parameters

(default parameters)

### Define numeric value domain



|                   |     |     |     |
|-------------------|-----|-----|-----|
| best values       |     |     |     |
| min               |     | max |     |
| 0                 | 100 | 100 | 100 |
| min               |     | max |     |
| acceptable values |     |     |     |

Run query

▶

@Web graphical user interface










Query Results (216)

Ontology: IC2ACV - Topics: Bioref-PM-PC-UFM-PS , Bioref-PM-PC-EX-PS , Bioref-PM , Bioref-PM-UFM , Bioref-PM-PC-PS , Bioref-PM-PC-UFM  
 Relation: Biomass glucose composition relation

Mandatory Desirable

| rank       | reliability score |   | Biomass<br>[Grasses and energetic plants ] | Glucose rate<br>[[0.000e+00;1.000e+02;1.000e+02;1.000e+02],%] | Biomass state     | Experience number |
|------------|-------------------|---|--|---|-------------------|-------------------|
| row 2_2317 | 1                 |    | Rice straw                                 | [5.333e+01;5.600e+01],%                                       | Untreated biomass | [2.000e+00],1     |
| row 2_2523 | 2                 |    | Bagasse                                    | [4.666e+01],%   | Untreated biomass | [3.000e+00],1     |
| row 1_2489 | 3                 |    | Rice straw                                 | [4.633e+01],%   | Untreated biomass | [1.000e+00],1     |
| row 0_2489 | 3                 |    | Rice straw                                 | [4.633e+01],%   | Untreated biomass | [0.000e+00],1     |
| row 5_2500 | 4                 |  | Rice straw                                 | [4.522e+01],%   | Untreated biomass | [5.000e+00],1     |
| row 0_2546 |                   |   |  |   |                   |                   |

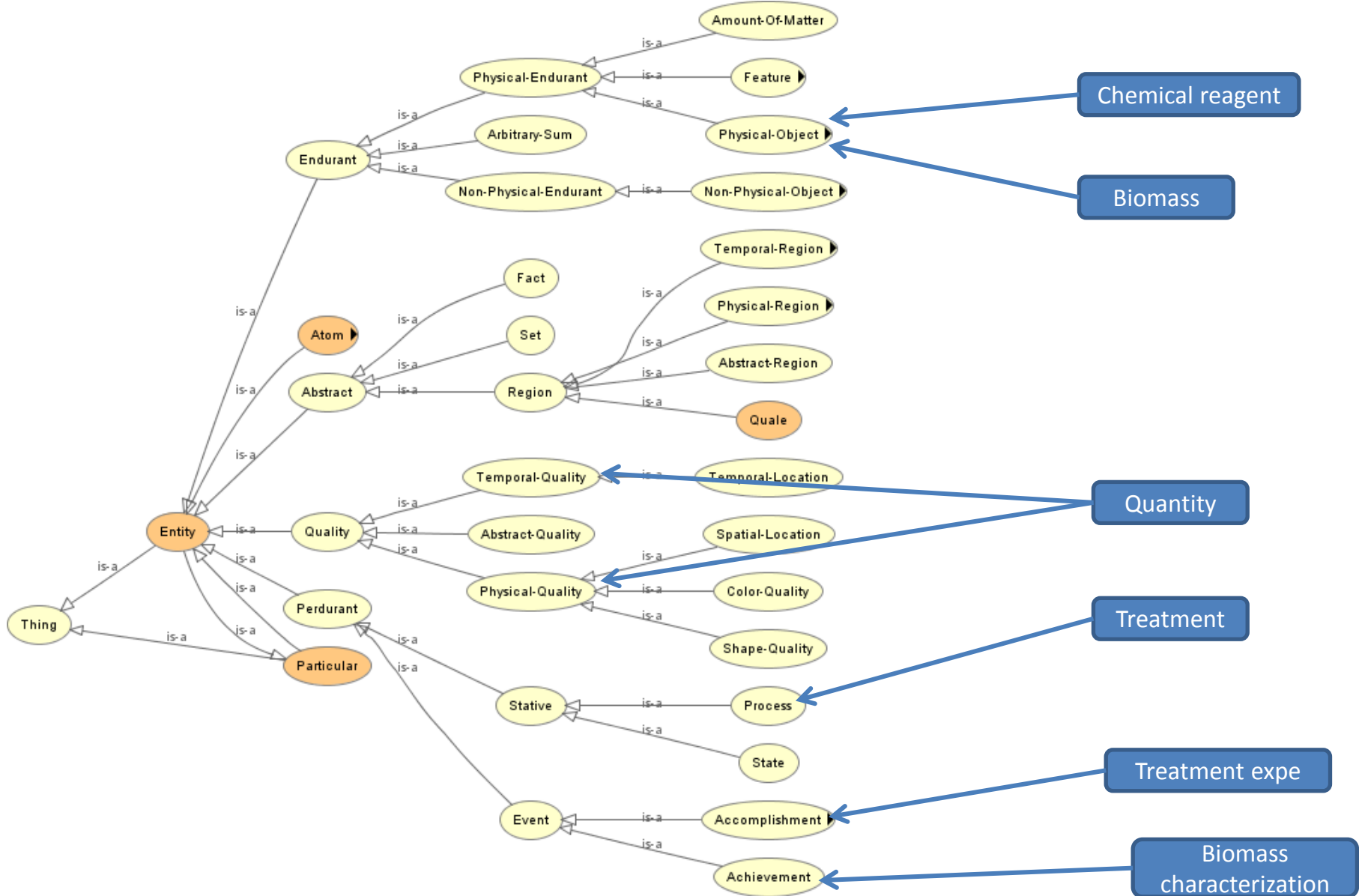
@Web graphical user interface



- A generic and reusable ontological model to capitalize experimental data
- Ontology consistency management
- Data reliability assessment
- Manual annotation guided by the ontology using text-mining assistant
- Flexible querying of annotated data combining 3 kinds of reasoning (specialization, fuzzy pattern matching, reliability satisfaction)

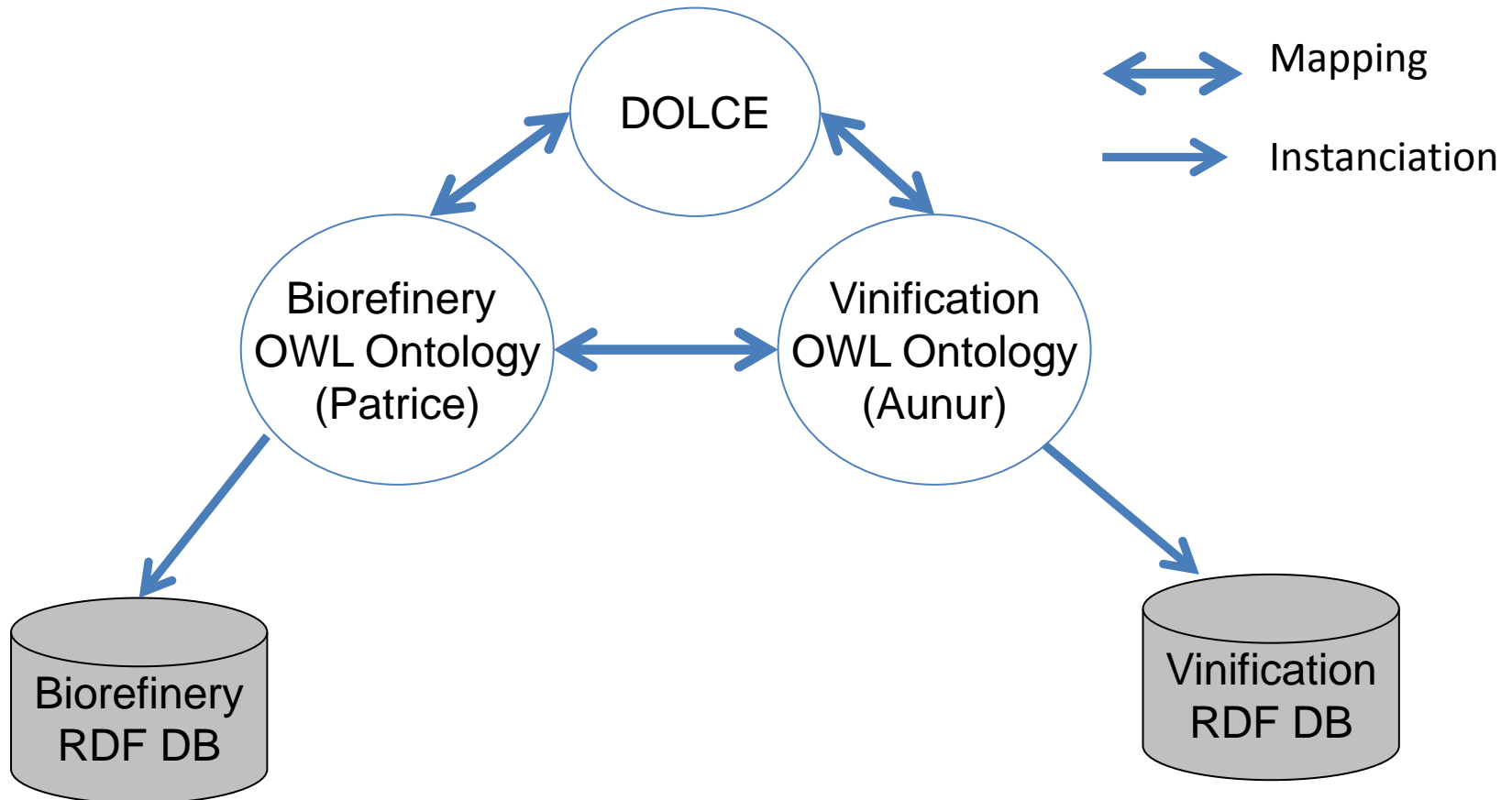


- CSV data file import
- RDF DB consistency management in case of ontology evolution
- Ontology mapping for Linked Open Data
- Assistant development to facilitate the manual annotation work
  - Text mining approach
  - Guidelines formalization using rules (OBDA approach)
- Extending core ontology to represent semantic links between n-ary relation concepts (temporal links, ...)





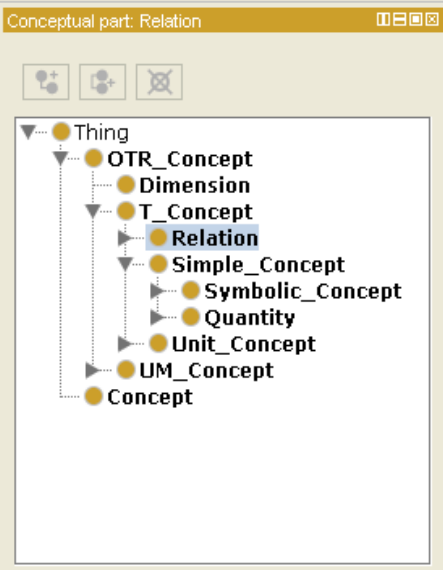
Which varieties of grapes having a “high” rate of tannin extraction from marc (vinification co-product) and “good” wine color parameters ?





# Modeling Guidelines associated with processes as rules

- Topic Bioref-PM, This Topic must contain experiences with only one milling followed by the enzymatic hydrolysis. It does not include a physico-chemical step but it can include a washing and separation step. (en)
- Topic Bioref-PM-PC-EX-PS, This Topic must contain experiences composed of a pre-milling step, then a physico-chemical treatment and an extrusion treatment and finally a press and separation step (washing and filtration) followed by the enzymatic hydrolysis step. (en)
- Topic Bioref-PM-PC-PS, This Topic must contain experiences composed of a least one pre-milling step, then a physico-chemical treatment and a washing and filtration step (washing and separation) and finally the enzymatic hydrolysis step. (en)
- Topic Bioref-PM-PC-UFM, This Topic must contain experiences composed of a pre-milling step, then a physico-chemical treatment followed by an ultrafine milling step (ball milling...) and finally the enzymatic hydrolysis step. This topic doesn't require a step of press and separation because it's a process with a low intake of effluent. The second milling step must give an "Output solid constituent size" smaller than 1 mm. (en)
- Topic Bioref-PM-PC-UFM-PS, This Topic must contain experiences composed of a pre-milling step, then a physico-chemical treatment followed by an ultrafine milling step (wet milling...) and a press and separation step (washing and filtration) and finally the enzymatic hydrolysis step. This topic requires a press and separation step because there are a lot of effluents in the physico-chemical step or because the milling is made with effluent. The second milling step must give an "Output solid constituent size" smaller than 1 mm. (en)



Terminological part: Relation

prefLabel :Relation  
 prefLabel :Concept compose  
 altLabel :Composed Concept

Changes:

Relation changes Argument changes Parameters

Elementary change : Add relation

New relation

New class :  Super class :

Arguments of the new relation

Number of arguments :

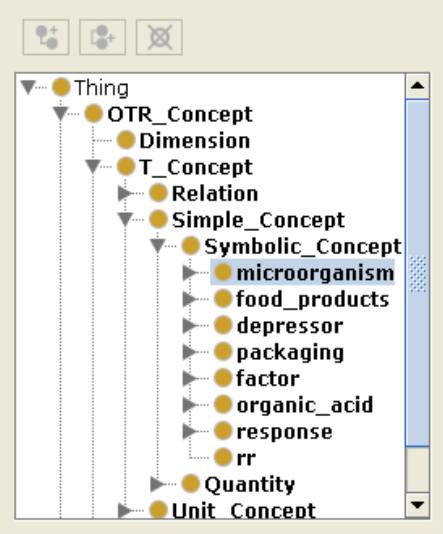
|             |   |  |  |                                |
|-------------|---|--|--|--------------------------------|
| Argument 1: | <input type="text" value="Symbolic_Concept"/> | <input type="text" value="packaging"/>       | <input checked="" type="radio"/> Important | <input type="radio"/> Optional |
| Argument 2: | <input type="text" value="Quantity"/>         | <input type="text" value="o2_permeability"/> | <input checked="" type="radio"/> Important | <input type="radio"/> Optional |
| Argument 3: | <input type="text" value="Quantity"/>         | <input type="text" value="thickness"/>       | <input checked="" type="radio"/> Important | <input type="radio"/> Optional |
| Argument 4: | <input type="text" value="Quantity"/>         | <input type="text" value="temperature"/>     | <input checked="" type="radio"/> Important | <input type="radio"/> Optional |
| Argument 5: | <input type="text" value="Choose"/>           | <input type="text" value="Choose"/>          | <input checked="" type="radio"/> Important | <input type="radio"/> Optional |

Terminology of the new relation

Preferred labels Alternative labels

Pref label 1 of relation:  Langue :

Conceptual part: microorganism



Terminological part: microorganism

prefLabel:Microorganism  
 prefLabel:microorganisme  
 altLabel:Strain  
 altLabel:micro-organisme::bactérie::germe::microbe::vir

Changes:

Relation changes Argument changes Parameters

Evolution strategies

**How to deal orphan concepts?**

Orphan concepts are :

- deleted
- reconnected to their parents
- reconnected to the root concept

**How to deal orphan properties?**

Orphan properties are :

- deleted
- reconnected to their parents
- left alone

**How to deal restrictions with undefined class in their definition?**

Restrictions are :

- deleted
- updated : replace the class representing the restricted range with its subclasses
- updated : replace the class representing the restricted range with one or more subclasses selected by the user

**How to deal restrictions with undefined property in their definition?**

Restrictions are :

- deleted
- updated : replace the property used in the restricted range with one property selected by the user

**How to deal instances whose concept is deleted?**

Instances are :

- deleted
- reconnected to the parents

**How to deal instances whose property is deleted?**

Instances are :

- deleted
- defined for the parent properties

**How to deal properties with undefined class in their domain/range?**

Undefined class is :

- deleted from the list of domains or co-domains
- replaced by its subclasses

**How to deal labels whose concept is deleted?**

Labels are :

- deleted
- reconnected to the subclasses of the deleted concept as alternative labels
- reconnected as alternative labels to one or more sub classes selected by the user

OK Reset





## Query Summary

| Query scope  |                          |
|--|--------------------------|
| Ontology   | MAPOPT                   |
| Topics   | "PackPermeability"       |
| Relation   | O2 Permeability_relation |
| Value domains wanted for attributes  |                          |
| <b>Mandatory</b>   |                          |
| (1) O2 Permeability : [5e-13 ; 1.27e-11 ; 1.5e-11 ; 1e-10] - unit : Mole per Meter per second per pascal |                          |
| Parameters   |                          |
| <input type="button" value="Run query"/>   |                          |

@Web graphical user interface

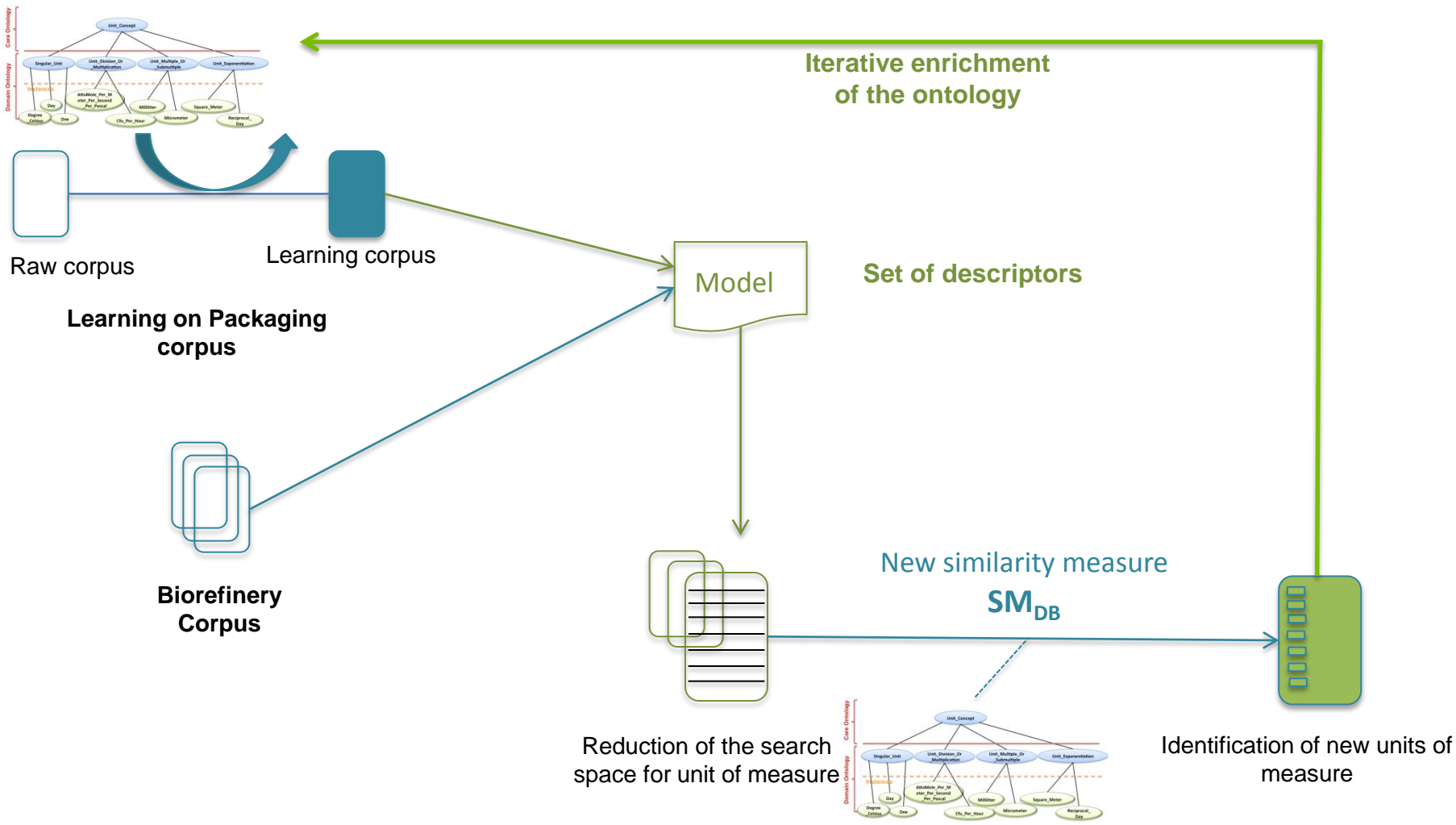


Ontology: MAPOPT - Topics: PackPermeability  
 Relation: O2 Permeability\_relation

Mandatory  Desirable

| rank       | reliability score |  | O2 Permeability<br>[[5.000e-13;1.270e-11;1.500e-11;1.000e-10],mol/m <sup>2</sup> s/Pa] | Temperature                                  | Thickness                | Relative Humidity        | Packaging      | Partial pressure difference                                    |                 |
|------------|-------------------|--|--|--|--------------------------|--------------------------|----------------|--|-----------------|
| row 0_318  | 1                 |  | •  | [2.950e+01;3.150e+01],cm3.mm.m-2.day-1.atm-1 | [2.400e+01;2.600e+01],°C | [2.000e+02;2.200e+02],µm | [-inf, +inf] % | Polylactic acid  | [1.000e+00],atm |
| row 1_318  | 1                 |  | •  | [2.290e+01;2.490e+01],cm3.mm.m-2.day-1.atm-1 | [2.400e+01;2.600e+01],°C | [2.000e+02;2.200e+02],µm | [-inf, +inf] % | (1wt%)Ag/Polylactic Acid                                       | [1.000e+00],atm |
| row 4_318  | 1                 |  | •  | [1.680e+01;1.880e+01],cm3.mm.m-2.day-1.atm-1 | [2.400e+01;2.600e+01],°C | [2.000e+02;2.200e+02],µm | [-inf, +inf] % | (5wt%)Cellulose nanocrystals/(1wt%)Ag/Polylactic Acid          | [1.000e+00],atm |
| row 0_2604 | 1                 |  | •  | [7.000e-01;1.800e+00],cm3.mm.m-2.day-1.atm-1 | [2.300e+01],°C           | [8.500e+01],µm           | [0.000e+00],%  | Chitosan/paper   | [1.000e+00],atm |
| row 5_318  | 1                 |  | •  | [1.160e+01;1.360e+01],cm3.mm.m-2.day-1.atm-1 | [2.400e+01;2.600e+01],°C | [2.000e+02;2.200e+02],µm | [-inf, +inf] % | (5wt%)Modified cellulose nanocrystals/(1wt%)Ag/Polylactic Acid | [1.000e+00],atm |
| row 3_318  | 1                 |  | •  | [1.320e+01;1.520e+01],cm3.mm.m-2.day-1.atm-1 | [2.400e+01;2.600e+01],°C | [2.000e+02;2.200e+02],µm | [-inf, +inf] % | (1wt%)Modified cellulose nanocrystals/(1wt%)Ag/Polylactic Acid | [1.000e+00],atm |

@Web graphical user interface





## Data

« Corpus Biorefinery »

- **243** scientific documents
- Unit terms extracted from the ontology : **36** terms

« Corpus Packaging »

- **115** scientific documents
- Unit terms extracted from the ontology : **211** terms

## Locate relevant information by learning

Reduction of « Corpus Biorefinery »

↓  
**90 %**

Reduction of « Corpus Packaging »

↓  
**86 %**

## Enrichment of the termino-ontological resource

Enrichment « OTR Biorefinerie »

↓  
**+ than 100 %**  
of new units

Enrichment «OTR Packaging»

↓  
**18 %**  
of new units