

# DFS TD - Synthesis Reaction Raw Data

Technical documentation for the data coming from reaction tests

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## Sum-up

Equipment / Scale	Reaction 25L (A and B)	Reaction 80L	Reaction 170L (France and Korea)	Reaction 2500L
<b>Data Sources</b>	<a href="#">ELN</a> , Raw Data on file share	<a href="#">ELN</a> , Raw Data on Google Drive	<a href="#">ELN</a> , Raw Data on file share	<a href="#">ELN</a> , Raw Data on Google Drive
<b>Raw Data File type</b>	xlsx	xlsx	xlsx	xlsx
<b>Scale Name on ELN</b>	FR-25L-A FR-25L-B	FR-80L	FR-170L KR-170L	FR-2500L
<b>Data Collection</b>	Talend: <ul style="list-style-type: none"><li>• J010_Download_Synthesis_LabServers</li></ul> Python : <ul style="list-style-type: none"><li>• download_synthesis_25L.py</li><li>• download_synthesis_25L_B.py</li></ul>	Talend: <ul style="list-style-type: none"><li>• R013_Download_Synthesis_gDrive_Reaction</li></ul>	Talend: <ul style="list-style-type: none"><li>• J010_Download_Synthesis_LabServers</li></ul> Python : <ul style="list-style-type: none"><li>• download_synthesis_170L.py</li><li>• download_synthesis_170L_KR.py</li></ul>	Talend: <ul style="list-style-type: none"><li>• R013_Download_Synthesis_gDrive_Reaction</li></ul>
<b>Parse</b>	Python: parse_synthesis_25L.py	Python: parse_synthesis_2500L.py	Python: <ul style="list-style-type: none"><li>• parse_synthesis_170L.py</li><li>• parse_synthesis_170L_KR.py</li></ul>	Python: parse_synthesis_2500L.py
<b>Compute</b>	Python: compute_synthesis_25L.py	Python: compute_synthesis_80L.py	Python: compute_synthesis_170L.py	Python: compute_synthesis_2500L.py
<b>BigQuery</b>	<i>Target tables:</i> <ul style="list-style-type: none"><li>• <i>raw_data_synthesis.ReactionDetails</i></li><li>• <i>raw_data_synthesis.ReactionSummary</i></li><li>• <i>raw_data_synthesis.ReactionMaterialBalance (table to be documented)</i></li></ul>			
<b>Mapping spreadsheet</b>	<a href="#">Mapping Spreadsheet</a>			

## Data Sources

- [ELN](#)
- Raw Data

## Data Collection

The talend jobs **J010\_Download\_Synthesis\_LabServers** and **J011\_Download\_Synthesis\_gDrive\_Reaction** extract the raw data files listed on the ELN table **synthesis\_raw\_data\_link** for which the field "synthesis\_equipment\_name" is the scale name, i.e. "FR-80L". For information of how these job works, check the following page :

Talend - Jobs - Synthesis - Download:

## Exemples

Lab servers source

- \\FRPH2-labpc-backup\labo\W-522649\DATAS DATALAKE
- \\FRPH2-LABPC-BACKUP\LABO\W-509931

Python files

- download\_filtration170L.py
- download\_synthesis25L.py

Output folders

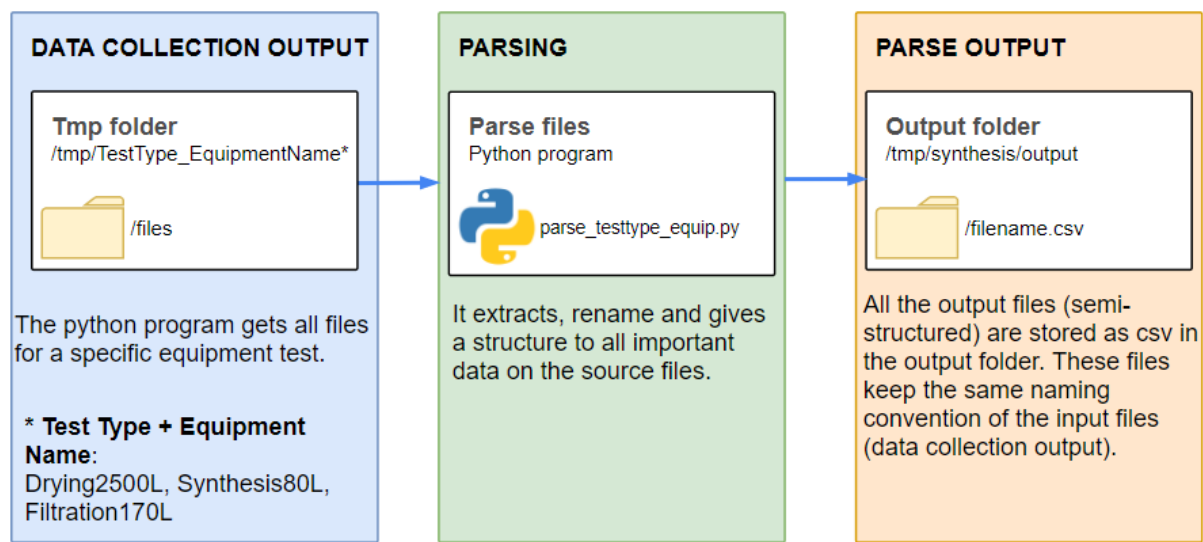
- D:\DATA\ENV\Rn\Silica\tmp\Synthesis25L
- D:\DATA\ENV\Rn\Silica\tmp\Synthesis170L

## Data Preparation

### Parse

The parsing python scripts extracts from the raw data files the needed columns.

## DATA PREPARATION - PARSE



### Columns List

For each sample, the script extracts the many fields from the raw data files and outputs a .csv file. For the mapping details, please refer to the sheet "Parse Mapping" on the Reaction Mapping spreadsheet (link to the spreadsheet on the Sum-up section).

The following columns extracted from the raw data file:

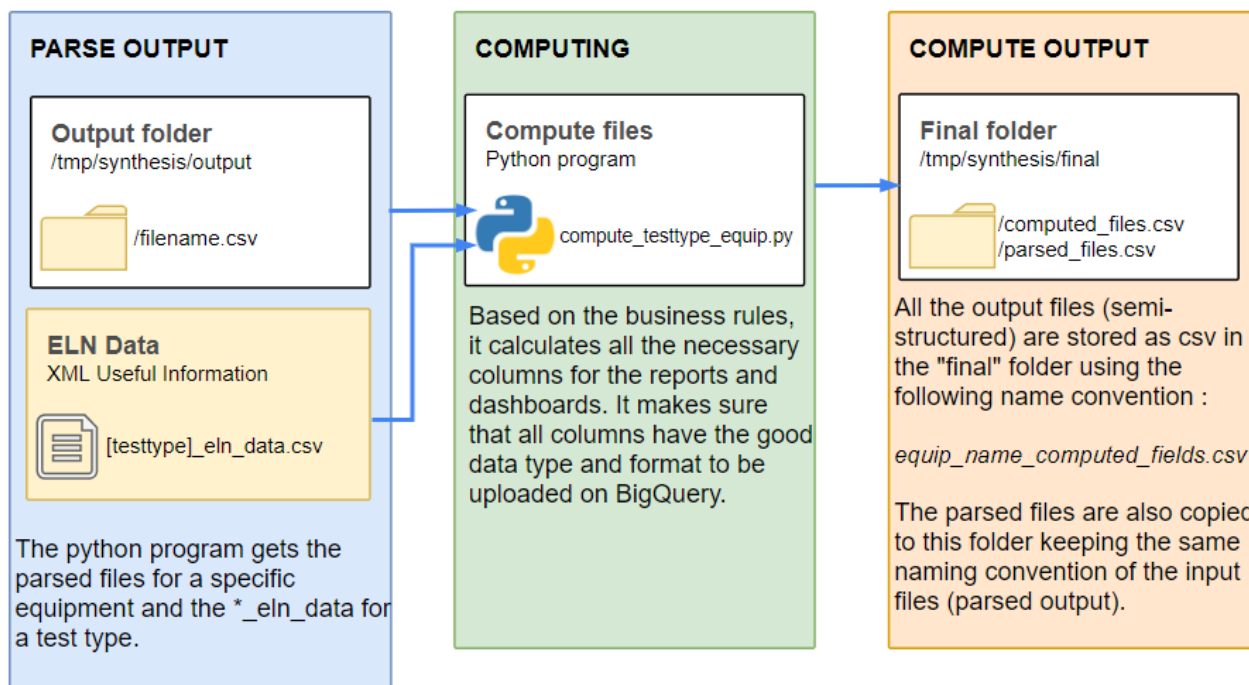
- unique\_id
- study\_id
- sample\_id
- operator
- reactor
- date
- time (in minutes)
- ph
- temperature
- acid\_mass\_one
- silicate\_mass
- additive\_mass
- acid\_mass\_two
- variable\_product\_mass (empty for 170L scale)
- percent\_acid\_one
- percent\_silicate
- percent\_additive
- percent\_acid\_two
- percent\_pump\_pH\_control
- percent\_variable\_product (empty for 170L scale)
- turbidity

### Compute

The compute python script uses as input the parsed .csv files previously created and the tables `synthesis_eIn_data` and `operating_procedure`. It computes the new columns and values from raw data and regenerates new files.

If the output files already exist the script will **NOT** replace them.

## DATA PREPARATION - COMPUTE



In the beginning of the script, for each product, we extract the following values for each product listed in the table **synthesis\_eln\_data** . Each of the following values will be used in later computations as constants:

Product	Variables
<b>Silicate</b>	<ul style="list-style-type: none"> <li>• density_silicate_eln = density_silicate (from ENL)</li> <li>• density_silicate               <ul style="list-style-type: none"> <li>◦ density_silicate extracted from ELN is replaced by the following computation:</li> <li>◦ <math>144 * \text{density\_silicate (from ELN)} / (144 + 0.035 * \text{density\_silicate (from ELN)} * \text{temperature\_max})</math></li> <li>◦ In the previous formula, temperature_max = maximum of the column [Temperature] from the raw data file</li> <li>◦ This correction is necessary for the computation of the total volume</li> </ul> </li> <li>• rp_silicate</li> <li>• silicate_qty</li> <li>• concentration_sio2</li> <li>• concentration_na2o</li> </ul>
<b>Water</b>	<ul style="list-style-type: none"> <li>• water_qty</li> <li>• density_water</li> <li>• concentration_water</li> </ul>
<b>Aluminate</b>	<ul style="list-style-type: none"> <li>• add_qty</li> <li>• density_add</li> <li>• concentration_add_al</li> <li>• concentration_add_na2o</li> </ul>
<b>Other</b>	<ul style="list-style-type: none"> <li>• other_qty</li> <li>• density_other</li> <li>• concentration_add_oo (product name = Other and compound name = Other)</li> <li>• concentration_add_ou (product name = Other and compound name = Unknown)</li> <li>• concentration_hplus_o (product name = Other and compound name = H+)</li> <li>• concentration_na2o_o (product_name = Other and compound name = Na2O)</li> <li>• nb_hplus_hplus_o</li> </ul>

<b>R66</b>	<ul style="list-style-type: none"> <li>• r66_qty</li> <li>• density_r66</li> <li>• concentration_add_rma (product name = R66 and compound name = 2-methylglutaric acid)</li> <li>• concentration_hplus_r (product name = R66 and compound name = H+)</li> <li>• nb_hplus_hplus_r</li> </ul>
<b>Sodium Sulfate</b>	<ul style="list-style-type: none"> <li>• sodium_sulfate_qty</li> <li>• concentration_sodium_sulfate</li> </ul>
<b>Sodium Hydroxide</b>	<ul style="list-style-type: none"> <li>• sodium_hydroxide_qty</li> <li>• concentration_sodium_hydroxide</li> <li>• density_sodium_hydroxide</li> </ul>
<b>Sulfuric Acid Concentrate</b>	<ul style="list-style-type: none"> <li>• h2so4_c_qty</li> <li>• concentration_h2so4_c</li> <li>• density_h2so4_c_eln = density_h2so4 (from ELN)</li> <li>• density_h2so4_c <ul style="list-style-type: none"> <li>◦ density_h2so4_c extracted from ELN is replaced by the following computation: <ul style="list-style-type: none"> <li>◦ <math>((-0.3119 * (\text{concentration\_h2so4\_c} * 100))^{** 2} + 61.569 * (\text{concentration\_h2so4\_c} * 100) - 1200.4) - (0.5133 * \text{temperature\_max}) / 1000</math></li> <li>◦ In the previous formula, temperature_max = maximum of the column [Temperature] from the raw data file</li> <li>◦ This correction is necessary for the computation of the total volume</li> </ul> </li> </ul> </li> <li>• nb_hplus_h2so4_c</li> </ul>
<b>Sulfuric Acid</b>	<ul style="list-style-type: none"> <li>• h2so4_d_qty</li> <li>• density_h2so4_d_eln = density_h2so4_d_eln (from ELN)</li> <li>• density_h2so4_d <ul style="list-style-type: none"> <li>◦ density_h2so4_d extracted from ELN is replaced by the following computation: <ul style="list-style-type: none"> <li>◦ <math>(\text{density\_h2so4\_d (from ELN)} * 1000 - 0.5133 * \text{temperature\_max}) / 1000</math></li> <li>◦ In the previous formula, temperature_max = maximum of the column [Temperature] from the raw data file</li> <li>◦ This correction is necessary for the computation of the total volume</li> </ul> </li> </ul> </li> <li>• concentration_h2so4_d</li> <li>• nb_hplus_h2so4_d</li> </ul>
<b>Nitric Acid Concentrate</b>	<ul style="list-style-type: none"> <li>• hno3_c_qty</li> <li>• density_hno3_c</li> <li>• concentration_hno3_c</li> <li>• nb_hplus_hno3_c</li> </ul>
<b>Nitric Acid</b>	<ul style="list-style-type: none"> <li>• hno3_d_qty</li> <li>• density_hno3_d</li> <li>• concentration_hno3_d</li> <li>• nb_hplus_hno3_d</li> </ul>
<b>Chlorhydric Acid Concentrate</b>	<ul style="list-style-type: none"> <li>• hcl_c_qty</li> <li>• density_hcl_c</li> <li>• concentration_hcl_c</li> <li>• nb_hplus_hcl_c</li> </ul>
<b>Chlorhydric Acid</b>	<ul style="list-style-type: none"> <li>• hcl_d_qty</li> <li>• density_hcl_d</li> <li>• concentration_hcl_d</li> <li>• nb_hplus_hcl_d</li> </ul>

**Molar masses** for the following elements are also defined and used in later computations (mm\_ stands for molar mass):

- mm\_na2o = 61.98
- mm\_h2so4 = 98.079
- mm\_sio2 = 60.084
- mm\_na2so4 = 142

- mm\_hcl = 36.46
- mm\_hno3 = 63.02
- mm\_hplus = 1.01

Next, we define the **activity on each pump** as follows:

- We first define "by default" activity on each pump:
  - acid\_one pump (concentrated acid) Sulfuric Acid Concentrate
  - silicate pump Silicate
  - additive pump Aluminate
  - acid\_two pump (diluted acid) Sulfuric Acid
- Next, from the table **operating\_procedure**, we extract the changes in the activity for each pump. The next table lists the products that can be present on each pump:



Any other element (other than those listed in the table for each pump) will not be considered for later computations

raw_mass_acid_one (conc)	raw_mass_silicate	raw_mass_additive	raw_mass_acid_two (dil)
<b>WIR811_Masse</b>	<b>WIR611_Masse</b>	<b>WIR711_Masse</b>	<b>WIR511_Masse</b>
Sulfuric Acid Concentrate (default)	Silicate (default)	Aluminate (default)	Sulfuric Acid (default)
Nitric Acid Concentrate		Other	Nitric Acid
Chlorhydric Acid Concentrate		R66	Chlorhydric Acid
Other			Other
R66			R66
Water			Water

For each sample, the compute scripts create **three different tables**:

## ReactionDetails

The **first table** is composed of the columns previously extracted from the raw data files and the new columns calculated during the execution.

Dataset : raw\_data\_synthesis\_mig

For the columns details, please refers to the sheets " **Details Mappings** " on the **Reaction Mapping** spreadsheet (link to the spreadsheet on the Sum-up section).

## ReactionSummary

The **second table** is composed of the new values computed from raw data. This is a atomic table and it aggregates the values by **unique\_id, study\_id and sample\_id** which represents one line per data raw file.

Dataset : raw\_data\_synthesis\_mig

For the columns details, please refers to the sheets " **Summary Mapping** " on the **Reaction Mapping** spreadsheet (link to the spreadsheet on the Sum-up section).

## ReactionMaterialBalance

*To be documented*

## Presentation

The raw data (already parsed) and the computed columns are created as tables on **BigQuery**. A Talend job is responsible to push all this data to a dataset called **raw\_data\_synthesis\_mig**.

## DATA PRESENTATION - UPLOAD TO BIGQUERY

