Using Boolean, Enumerated and Inter-sample Custom Fields

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Agenda

- Custom Field Examples
  - Boolean Fields
    - and/or statements
    - use as: position
  - Enumerated Fields
  - Functions
    - REPLACE
    - ROUND
Boolean Type
Custom Fields

Definition: A custom field with Boolean data type is a mathematical formula that returns one or two possible expressions.

- We create a Boolean CF that tells us if an amount is **Low** or **Not Low**: 
  \[ \text{OK\_ThBr} = \text{GT}(C\text{CompRef1}[\text{Amount}], 10) \]
Create Boolean CF: OK_ThBr

- OK_ThBr = GT(CCompRef1[Amount], 10)

Boolean Functions:
- ENUM: Enumeration
- EQ: Equal
- GT: Greater than
- GTE: Greater than or equal
- LT: Less than
- LTE: Less than or equal
- NEQ: Not equal
- RANGE: Range
- EQI: Equal, case insensitive
- NEQI: Not equal, case insensitive

We will do the same for Caffeine

OK_Caf = GT(CCompRef2[Amount], 20)
In Review enter CCompRef in the Component table.

Process Sample in Review.

- OK_Caf: 8.087 Low
- OK_ThBr: 26.118 Not Low
Instead of the values (10, 20) we use CConst1

\[ \text{OK}_1 = \text{GT}(\text{CCompRef1}[\text{Amount}], \text{CConst1}) \]
Process
Boolean CF with CConstn

In Review enter CCompRef1 and CConst1

<table>
<thead>
<tr>
<th>Name</th>
<th>Retention Time (min)</th>
<th>RT Window (min)</th>
<th>Y Value</th>
<th>X Value</th>
<th>Rt</th>
<th>Type</th>
<th>CCompRef1</th>
<th>CCompRef2</th>
<th>CCompRef3</th>
<th>CConst1</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.717</td>
<td>0.145</td>
<td>Area</td>
<td>Amount</td>
<td>Linear</td>
<td>Single</td>
<td>ThBr</td>
<td>10.000000000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>4.047</td>
<td>0.654</td>
<td>Area</td>
<td>Amount</td>
<td>Linear</td>
<td>Single</td>
<td>Car</td>
<td>20.000000000</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Process Samples

OK_CConst1 Low
Not Low
Create Boolean CF with: And, RANGE statement

- When you want to combine the two statements in a RANGE, you can create CF:

\[ \text{OK} = \text{RANGE}(\text{CCompRef1[A]} \text{Amount}, 10, 14) \& \text{RANGE}(\text{CCompRef2[A]} \text{Amount}, 20, 30) \]

Where the operators: \& = \text{AND}, 1 = \text{OR}
Process Boolean CF with:
And, RANGE statement

OK = RANGE(CCompRef1[Amount], 10, 14) & RANGE(CCompRef2[Amount], 20, 30)
Enumerated Custom Fields

Definition: A custom field with Enumeration is a data type with one or more Boolean expressions

- A Boolean always has two statements: Pass or Fail
  Example: $\text{OK}\_\text{ThBr} = \text{GT}(\text{CCompRef1}\[\text{Amount}\], 10)$

- A Enumeration has more than two possible answers
  Example: Low/Good/High

- The same functions and operators apply as in Boolean

- An example Custom Field is:
  $\text{OK}\_\text{Enum} = \text{ENUM}(\text{LT}(\text{CCompRef1}\[\text{Amount}\], 9), \text{RANGE}(\text{CCompRef1}\[\text{Amount}\], 9, 14), \text{GT}(\text{CCompRef1}\[\text{Amount}\], 14))$
Create Enumeration CF

\[
\text{ENUM(LT(CCompRef1[Amount], 9), RANGE(CCompRef1[Amount], 9, 14), GT(CCompRef1[Amount], 14))}
\]

Cut and Paste a Calculation

**TIP**

To make it more easier, you can use cut and paste to or from copy a word editor.
Create Enumeration CF: OK_Enum

OK_Enum=ENUM(LT(CCompRef1[Amount],9),
RANGE(CCompRef1[Amount],9,14),
GT(CCompRef1[Amount],14))

OK_Enum
Low
Good
High

Use As

If you specified a data type as either ENUM or BOOL in the Data and Type Selection page and a formula is created, select how you want to produce the result of the calculation:
Use As

- **Use As**
  - **Position**
    - The result of the formula is treated as a number corresponding with the Value column of the Translation table.
  - **Text**
    - The result of the custom field formula is treated as a text string.
  - **Value**
    - The result of the custom field formula is treated as a numerical value.

Final_Amount

Final_Amount = Amount * Low_Amount

GT(Amount, 9)
Final_Amount = Amount * Low_Amount

<table>
<thead>
<tr>
<th>Name</th>
<th>Type</th>
<th>Field Type</th>
<th>Width</th>
<th>Precision</th>
<th>Min</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>Final_Amount</td>
<td>Real(G6)</td>
<td>Peak</td>
<td>12</td>
<td></td>
<td>1000</td>
<td>10000</td>
</tr>
<tr>
<td>Low_Amount</td>
<td>Boolean</td>
<td>Peak</td>
<td>6</td>
<td></td>
<td>0</td>
<td>1000</td>
</tr>
<tr>
<td>OK_Car</td>
<td>Boolean</td>
<td>Peak</td>
<td>7</td>
<td></td>
<td>0</td>
<td>1000</td>
</tr>
<tr>
<td>OK_Burn</td>
<td>Boolean</td>
<td>Peak</td>
<td>4</td>
<td></td>
<td>0</td>
<td>1000</td>
</tr>
<tr>
<td>OK_THOR</td>
<td>Boolean</td>
<td>Peak</td>
<td>7</td>
<td></td>
<td>0</td>
<td>1000</td>
</tr>
<tr>
<td>SampleName</td>
<td>Text</td>
<td>Sample</td>
<td>32</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SampleWeight</td>
<td>Real(G6)</td>
<td>Sample</td>
<td>8</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Final_Amount = Amount * Low_Amount

<table>
<thead>
<tr>
<th>Amount</th>
<th>Final_Amount</th>
<th>Low_Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.087</td>
<td>0.000</td>
<td>Too Low</td>
</tr>
<tr>
<td>26.447</td>
<td>26.447</td>
<td>Good</td>
</tr>
</tbody>
</table>
Enum Use As functionality

- "Use as" functionality introduced in Empower2: Field
  - Available only when Data Source is calculated

  - Items listed in the Enum Definition table are interpreted either as Empower fields (incl. Cust. Fields) or as strings
    - "fc" represents a formula calculation
    - Entries without "fc" are regarded as strings

  - If the result of this field is a number, it gets rounded and stored as a string
  - Result of this custom field can be used in another formula for a text comparison

Enum Use As Example

- **Use same functions as in Boolean custom fields to determine conditions:**
  - 1. If signal to Noise is under LOD: \( \text{LT}([s/n],100) \)

  - 2. If Signal to Noise is low: \( \text{RANGE}([s/n],100,200) \)

  - 3. If Signal to Noise is OK: \( \text{GT}([s/n],200) \)

- **Complete formula:**
  - \( \text{ENUM} \left( \text{LT}([s/n],100), \text{RANGE}([s/n],100,200), \text{GT}([s/n],200) \right) \)
**Enum Use As Example**

- Use translation table to define effects of different conditions:
  1. Field should contain no value: \(-1 \times 5000\) (fc)
  2. A warning will be posted: Low S/N-Investigate
  3. The Amount shall be reported: Amount (fc)

**Difference between Caf and ThBr**

- Peak Grouping calculates the sum of Components
- To calculate the difference we have to create CF:

  \[ \text{Extr}_\text{Amount}\_\text{Diff} = \text{Caf}[\text{Extr}_\text{Amount}] - \text{ThBr}[\text{Extr}_\text{Amount}] \]
In Review Process

Extr_Amount_Diff

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CCompRef(CCF) calculations

- Here the drawbacks are
  - Same values appear for both components
  - For every difference a new custom field is required
- To overcome this we can create a CF:
  \[ \text{Extr}_\text{Amount}_\text{Diff}_\text{CCR} = \text{CCompRef1}[\text{Extr}_\text{Amount}] - \text{CCompRef2}[\text{Extr}_\text{Amount}] \]
- Define the components as CCompRef 1 or CCompRef 2 in the component table
Create CF:
Extr_Amount_Diff_CCF

Extr_Amount_Diff_CCR = CCompRef1[Extr_Amount] - CCompRef2[Extr_Amount]

Process CF:
Extr_Amount_Diff_CCF

Extr_Amount_Diff CCR: 0.047
Extr_Amount_Diff CCF: 0.047
To display Extr_Amount_Diff_CCR the same way as in peak grouping. Create a dummy peak group and select CCompRef on the group line.

Replace

When the contents of a particular field are blank (or empty), you can specify a value to be displayed or used instead.

Example

\[ CF = \text{LTE}(\text{REPLACE}(\text{Amount}, 0), \text{CConst1}) \times -60002 + \text{GT}(\text{REPLACE}(\text{Amount}, 0), \text{CConst1}) \times \text{Amount} \]

Note: -60002 = Not Detected
We still have two columns

- To have one column we create a CF:
  \[ \text{Final Amount} = \text{REPLACE(Extr Amount Diff CCR, Extr Amount)} \]

- When Extr_Amount_Diff_CCR column is empty, the content of Extr_Amount is in the Final_Amount column.

- Otherwise the Extr_Amount_Diff_CCR value will be in the Final_Extr_Amount column.

<table>
<thead>
<tr>
<th>No.</th>
<th>Name</th>
<th>RT (min)</th>
<th>Area (µV*sec)</th>
<th>% Area</th>
<th>Height (µV)</th>
<th>Amount</th>
<th>Extr_Amount</th>
<th>Extr_Amount_Diff_CCR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ThrGr</td>
<td>1.79</td>
<td>261217</td>
<td>6.47</td>
<td>63238</td>
<td>13.381</td>
<td>0.852</td>
<td>0.647</td>
</tr>
<tr>
<td>2</td>
<td>Cat</td>
<td>4.11</td>
<td>3777823</td>
<td>63.53</td>
<td>883231</td>
<td>23.063</td>
<td>1.539</td>
<td>0.647</td>
</tr>
<tr>
<td>3</td>
<td>Extr_Amount_Diff_CCR</td>
<td>261217</td>
<td>6.47</td>
<td>63238</td>
<td>0.852</td>
<td>0.647</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Custom Calculation**

**Special Values**

<table>
<thead>
<tr>
<th>Value</th>
<th>Translation (displayed)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-50000</td>
<td>Blank Cell (No value is displayed)</td>
</tr>
<tr>
<td>-60000</td>
<td>ND</td>
</tr>
<tr>
<td>-60001</td>
<td>N.D.</td>
</tr>
<tr>
<td>-60002</td>
<td>Not Detected</td>
</tr>
<tr>
<td>-60003</td>
<td>N/D</td>
</tr>
<tr>
<td>-60004</td>
<td>NA</td>
</tr>
<tr>
<td>-60005</td>
<td>Not Found</td>
</tr>
<tr>
<td>-60006</td>
<td>Below Detection Limit</td>
</tr>
<tr>
<td>-60007</td>
<td>BDL</td>
</tr>
<tr>
<td>-60008</td>
<td>Below Peak Quantitation Limit</td>
</tr>
<tr>
<td>-60009</td>
<td>BPQL</td>
</tr>
</tbody>
</table>

Note: All or Nothing must be enabled for the translation to take place.
REPLACE:
Final_Amount

Final_Amount = REPLACE(Extr_Amount_Diff_CCR, Extr_Amount)

REPLACE:
Final_Amount
Round Function

- The rounding function allows you to round large numbers in calculations.
- You can use the round function in the New Custom Field Wizard – Formula Entry page.

ROUND (field,#)

For example:
- ROUND(25.678,0) will be rounded to 26
- ROUND(256575.36,3) will be rounded to 257000
- ROUND(25.657536,-3) will be rounded to 25.658
Exercise

- USE

—Exercise 2 Project