In C6 and See3 there was a recipe generation stored procedure which was part of the Oracle CM database. This seemed to work well, so we never tried to recapitulate the function, but just called the stored procedure as required.

Generally the problem of turning a screen into a recipe is relatively straightforward, except for buffering solutions.

A recipe is made up in a fixed volume; by default we make up 1mL, which is then scaled up or down as needed.

Any “spare” space in 1 mL is filled with water

Each condition is treated independently, until the all the conditions in a screen have been translated from factors to stocks and volumes.

For each condition:

For each factor in the condition, find out if there exists a stock of that chemical

If there is a stock, calculate how much one would need of that stock to create the required concentration

Eg.

Take a condition

0.2 M Magnesium chloride, 20 w/v Polyethylene glycol 3350, 0.1 tris chloride pH 8.5

Factors are

1. 0.2 M magnesium chloride
2. 20 w/v polyethylene glyol 400
3. 0.1 M tris chloride pH 8.5

**For factor 1**

Say we find two matching stocks – 1 M magnesium chloride, and 2 M magnesium chloride

If we were to use the 1 M stock, we would need 0.2 M / 1 M x 1 mL (default volume) or 0.2 mL

If we were to use the 2 M stock, we would need 0.2 M / 2 M x 1 mL or 0.1 mL

(note that if our stock were 0.1 M magnesium chloride we would need 0.2 M / 0.1 M x 1 mL or 2 mL – which is impossible – this is called an overflow, and there would be an error statement passed to the user. The error message would minimally contain the information “ 0.1 M magnesium chloride is insufficiently concentrated”. After calculating the rest of the factors, further information could be added, see below.

We use the least concentrated stock that will not overflow for the recipe generation.

**For factor 2**

Say we have a matching stock of 80 w/v Polyethylene Glycol 400

We would need 20 w/v / 80 w/w x 1 mL or 0.25 mL

Confusingly, some polyethylene glycols (PEGs) are given in v/v not w/v. Say we had an 80 v/v stock, rather than 80 w/v. The easiest would be to give the user a warning - Polyethylene glycol 400 stock is v/v. Should we assume v/v = w/v? (y/n). If yes, then just continue as above. If n, then we have to multiply the stock by the density (which should be one of the attributes of the chemical). Density of PEG 400 = 1.13 g/mL, so the calculation becomes

20 w/v / (80 v/v \* 1.13) or 0.221 mL of the 80 v/v stock.

For factor 3

The following holds for buffering chemicals with a single pKa, or with pKas which are separated by more than two pH units.

If we have a matching stock (say 1 M tris HCl pH 8.5), then we proceed as in any other case

* 1. M / 1 M x 1 mL = 0.1 mL of the 1 M tris chloride pH 8.5 stock

If there is no exact match of stock, but there is a suitable stock <= 0.1 pH unit away, then that is used instead – here a stock of 1 M tris chloride pH 8.6 would be a suitable match. (this should be notified to the user).

More likely, there will be a pair of stocks that flank the pH value we desire (if more than one pair, then we take the closest flanking pair), and we use the Henderson Hasselbach (HH) approximation to determine the ratio of the pair to use. The flanking pair need to have the same concentration. Assume we have two 1 M tris chloride stocks, one at pH 7 and one at pH 9.

From above, we know that we need a total of 0.1 mL of 1 M tris chloride stock. HH approximation tells us that we would need 0.21 of the pH 7 stock mixed with 0.79 of the pH 9 stock, as we need 0.1 mL in total we would use 0.021 mL of 1 M tris chloride pH 7 and 0.079 mL of 1 M tris chloride pH 9

(the HH calculation is captured in the “buffer\_screen\_2021”) spreadsheet.

In the case where the buffering chemical is made up of two or more different components, then we use a lookup curve to estimate the proportions of the flanking stocks to use. The lookup curves were derived experimentally, and are also available in the “buffer\_screen\_2021” spreadsheet.

Once all conditions that are being translated to a recipe have been processed, check the list of stocks. If there is more than one stock of the same chemical then go back to the conditions that use the multiples, and find the single stock that will work in for each factor, and redo the calculations for the conditions using only that stock.