compute function:

dt-record:

1. sml=quantity of suppressor when addition completed

2.sv=total volume of suppressor added when addition completed

3.sc=sml/sv

4.vv=base volume

5.compute x value of output curve at y=evaluation ratio using cubic spline interpolation. let result be sv1.

6.calibration factor z=sc/(1+vv/sv1);

$$z = \frac{C_S}{1 + \frac{V_b}{V_S(R)}}$$

dt-analysis:

1.vv=base volume

2. compute x value of output curve at y=evaluation ratio using cubic spline interpolation. let result be spv.

3.if calibration factor z is given, sample suppressor concentration spc=z*(1+vv/spv).

4.if calibration factor z not given, compute z from another dt-record file with evaluation ratio in this setting. sample suppressor concentration spc=z*(1+vv/spv).

$$C_{sp} = z\left(1 + \frac{V_b}{V_{sp}(R)}\right)$$

lat-record:

1.compute the cubic spline interpolation of output curve.

2.compute the expression of derivative of cubic spline interpolation.

3.compute the last intersection of derivative curve and line y=thres. default value of thres is -0.05. the x value of result is intercept concentration.

lat-analysis:

1.spv=total volume of solution when sample addition completed.

2.spv0=total volume of sample added.

3.intercept Q itq=charge value when suppressor addition completed

4.select data points of accelerator addition from output curve and do linear fitting. result is y=k*x+b.

5.sample accelerator concentration spc=-(itq-b)/k*spv/spv0.

$$C_{sp} = \frac{V_{total}(b - Q_{it})}{V_{sp}k}$$

rc-record:

1.Q=evaluation ratio*charge of last suppressor-accelerator addition step.

2.compute x value of output curve at y=Q, using cubic spline interpolation. result is leveler concentration.

rc-analysis:

1.spv=total volume of solution when sample addition completed

2.spv0=total volume of sample added

3.q=charge of last sample addition step.

4.read another rc-record file, q0=charge of last step of this rc-record file.

5.compute leveler concentration of this rc-record file with evaluation ratio=q/q0. result is lc.

6.sample leveler concentration spc=lc*spv/spv0.

$$C_{sp} = \frac{C_L V_{total}}{V_{sp}}$$

sar-record:

1.compute x value of the output curve at y=evaluation ratio, result is sconc.

2.ac=accelerator concentration of solution when suppressor-accelerator addition completed.

3.sc=suppressor concentration of solution when suppressor-accelerator addition completed.

4.aconc=sconc*ac/sc.

5.for each output curve, repeat step 1-4, and result are the data points (aconc,sconc)

6.do linear fitting to data points (aconc,sconc). result is the sa-relation s=k*a+b.

sar-analysis:

1.vv=base volume

2.spvend=volume of sample added

3.compute sa-relation line from another sar-record file, result line s=k0*a+b0.

4.select the output curve which is zero accelerator concentration from this sar-record file. let this output curve be snq0.

5.do linear fitting to second output curve (correspond to accelerator addition). result line is y=k*x+b.

6.compute x value of first output curve (correspond to sample addition) at y=evaluation ratio using cubic spline interpolation. result is spv.

7.let ac=0.

8.sc=k0*ac+b0*(vv/spv+1)

9.compute y value of curve snq0 at x=sc/(vv/spvend+1) using cubic spline interpolation. result is tmp.

10.ac=(b-tmp)/k*(vv/spvend+1);

11.repeat step 8-10 n times. n=3 by default.

12.sample suppressor concentration is sc, sample accelerator concentration is ac.

$$C'_{Ssp} = k_{SAR} C'_{Asp} + \frac{b_{SAR}}{G} \left(\frac{V_b}{V_{sp}(R)} + 1 \right)$$

$$C'_{Asp} = \frac{b_A - q(C_S = C'_{Ssp}, C_A = 0)}{k_A}$$

$$G = \frac{V_b}{V_{sp}} + 1$$

$$C_{Ssp} = G C'_{Ssp}$$

$$C_{Asp} = GC'_{Asp}$$

pal-record:

1. compute x value of the output curve at y=evaluation ratio, result is leveler concentration.

pal-analysis:

1.spv=total volume of solution when sample addition completed

2.spv0=total volume of sample added.

3.lml=quantity of leveler when leveler addition completed.

4.nq=normalized charge when sample addition completed.

5. compute leveler concentration from another pal-record file with evaluation ratio=nq. result is lc.

6.sample leveler concentration spc=(lc*spv-lml)/spv0.

$$C_{sp} = \frac{C_L V_{total} - m_L}{V_{sp}}$$

lrt-record:

1.do linear fitting to output curve, result line is y=k*x+b, this is the regression line.

lrt-analysis:

1.spv0=total volume of sample added.

2.lml=quantity of leveler when leveler addition completed

3.nq=normalized charge when leveler addition completed

4.spv=total volume of solution when leveler addition completed

5.read another lrt-record file and compute regression line y=k0*x+b0.

6.ignore first n points of output curve and do linear fitting, result fitting line is y=k*x+b. n=3 by default.

7.sample leveler concentration spc=((nq-b0)/k*spv-lml)/spv0.

$$C_{sp} = \frac{V_{total}(q - b_{std})}{kV_{sp}} - \frac{m_L}{V_{sp}}$$