Simulation of Nd-Fractionation (basic mode)

A) Definitions of ratios (uni-directional [light/heavy]):

File:simulREDemo.mcd

$R_1 := 1.14179$ $\quad R_3 := \frac{1}{0.236421}$ $\quad R_N := \frac{1}{0.7219}$ $\quad R_3 = 4.229743$ $\quad R_N = 1.385233$ $\quad q := 1, 0.95 .. 0.25$

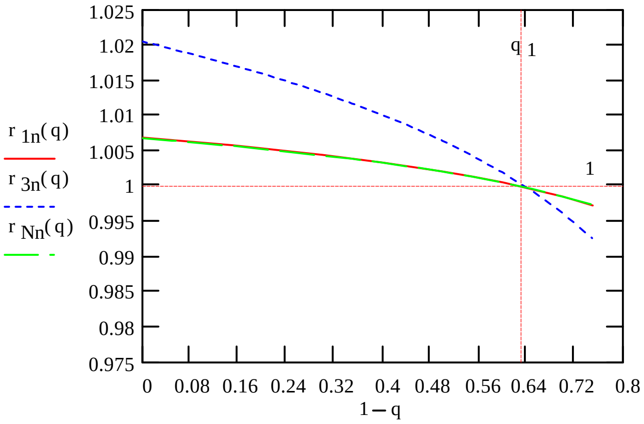
$\beta_1 := \sqrt{\frac{144}{142}}$ $\quad \beta_3 := \sqrt{\frac{150}{144}}$ $\quad \beta_N := \sqrt{\frac{146}{144}}$ $\quad X_1 := \frac{\beta_1 - 1}{\beta_1}$ $\quad X_N := \frac{\beta_1 \cdot \beta_N - 1}{\beta_1 \cdot \beta_N}$ $\quad X_3 := \frac{\beta_1 \cdot \beta_3 - 1}{\beta_1 \cdot \beta_3}$

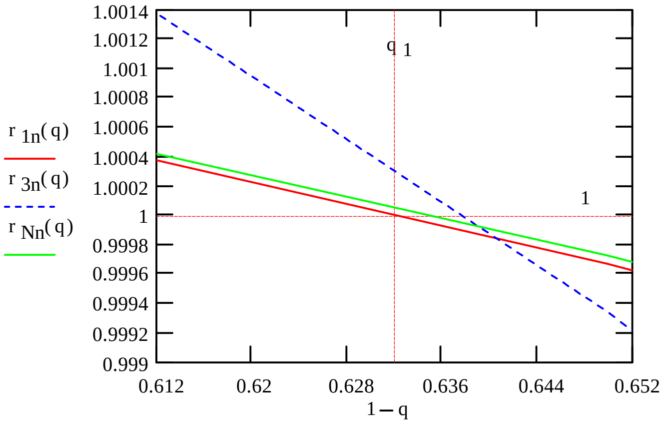
B) Assumption : Emission profiles follow Rayleigh distillation law:

$r_1(q) := R_1 \cdot \beta_1 \cdot q^{X_1}$ $\quad r_3(q) := R_3 \cdot \frac{R_1}{r_1(q)} \cdot \beta_1 \cdot \beta_3 \cdot q^{X_3}$ $\quad r_N(q) := R_N \cdot \frac{R_1}{r_1(q)} \cdot \beta_1 \cdot \beta_N \cdot q^{X_N}$ $\quad q_1 := 1 - \frac{1}{e}$

$r_{1n}(q) := \frac{r_1(q)}{R_1}$ $\quad r_{3n}(q) := \frac{r_3(q)}{R_3}$ $\quad r_{Nn}(q) := \frac{r_N(q)}{R_N}$ $\quad q_a := q_1 - 0.02$

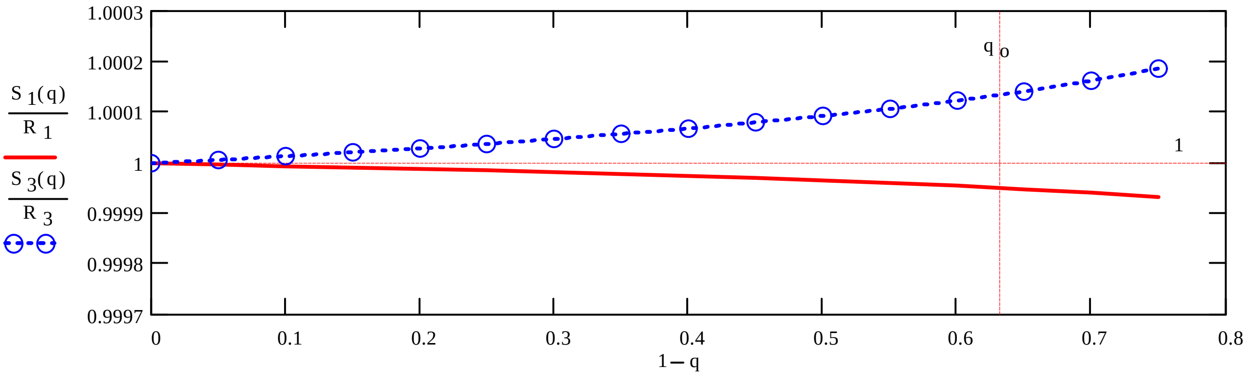
$q_e := q_1 + 0.02$





C) Fractionation correction, using Exponential law algorithms:

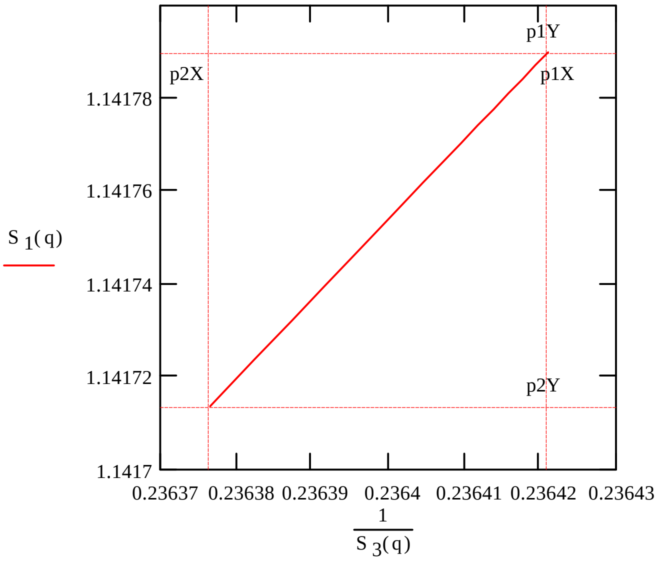
$A_3 := \frac{\ln(\beta_3)}{\ln(\beta_N)}$ $\quad A_1 := \frac{\ln(\beta_1)}{\ln(\beta_N)}$ $\quad S_1(q) := r_1(q) \cdot \left(\frac{R_N}{r_N(q)}\right)^{A_1}$ $\quad S_3(q) := r_3(q) \cdot \left(\frac{R_N}{r_N(q)}\right)^{A_3}$ $\quad q_o := 1 - \frac{1}{e}$



Please note: a) The Expo law 'overcompensates' the fractionation of the ratio with Δm=2, and
b) it does not fully compensate the fractionation of the ratio with Δm=6 .
With the given assumptions, *one therefore will inevitably obtain*
(a small) ***"residual correlation"*** *(Caro et al.) between these two ratios .*
In other words: The Exponential law is, under the given assumptions, not the 'most appropriate' correction algorithm (it is, however, fairly convenient).

D) Predicted "Residual correlation" :

Limits >>> $p1X := \frac{1}{S_3(1)}$ $p1Y := S_1(1)$ $p2X := \frac{1}{S_3(0.25)}$ $p2Y := S_1(0.25)$



$Slope := \frac{p1Y - p2Y}{p1X - p2X}$ $Slope = 1.72$

This slope is very similar to the experimental data of G.Caro et al. (Nature 423 (2003)).

It may, hence, be assumed, that their Nd data are evaporating according to the Rayleigh distillation law.

Please note: A plot of two unidirectionally defined ratios would exhibit a negative slope under the given assumptions !

Remark: I belief it would be worthwhile to repeat the evaluation of the Paris data, using the Rayleigh type correction algorithms.