Pseudocode for the MCA/LMA optimisation approach

Davis Marshall Todt

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procedure $f6p\_optimization$
    $p_1, p_2, p_3, p_4 \leftarrow mc\_approach(\ )$
    $optimal\_f6p \leftarrow minimize(objfunct, p_1, p_2, p_3, p_4)$
    $return\ \frac{1}{optimal\_f6p}$ \\optimal F6P value is returned to the user

procedure $mc\_approach(\ )$
    $Parameterlist \leftarrow emptylist$ \\for storing all generated parameter sets
    $F6Plist \leftarrow emptylist$ \\for storing all f6p values

    for i *in* $range(2000)$ **do**
        $p_1, p_2, p_3, p_4 \leftarrow gen\_random()$ \\generate random values between 0 and 1 (arbitrary range)
        $max\_f6p\_value \leftarrow \frac{1}{objfunct(p_1,p_2,p3,p4}$ \\perform simulation and store f6p value
        $F6Plist[i] \leftarrow max\_f6p_value$
        $Parameterlist[i] \leftarrow parameter\ set\ p_1, p2, p3, p4$
        $sort\_ascending(F6Plist, Parameterlist)$
        $return\ Parameterlist[1999]$ \\return optimum parameter set for use in 'minimize' function

procedure $objfunct(p_1, p_2, p_3, p_4)$
    $p_1, p_2, p_3, p_4 \leftarrow normalize(p_1, p_2, p_3, p_4)$
    $set\_model\_parameters(objfunct, p_1, p_2, p_3, p_4)$
    $simulate(\ )$
    $max\_f6p\_value \leftarrow extract\ max\ f6p\ from\ the\ simulation$
    $return \frac{1}{max\_f6p\_value}$ \\return the inverse of the maximum for subsequent minimization

procedure $normalize(p_1, p_2, p_3, p_4, Enzyme\_total)$
    $Enzyme\_total \leftarrow 0.4995$ \\total enzyme concentration

    for i *in* $range(4)$ **do**
        $p_i \leftarrow Enzyme\_total * \frac{pi}{\sum_{j=1}^{4} pj}$ \\normalize parameters to add up to 'Enzyme_total' constraint

    $return\ p_1, p_2, p_3, p_4$

procedure $set\_model\_parameters(p_1, p_2, p_3, p_4)$
    $Set\ appropriate\ parameters\ in\ the\ model\ to\ p_1, p_2, p_3, p_4$

procedure $simulate(\ )$
    $Simulate\ using\ the\ model\ 'kouril3'\ for\ production\ of\ F6P\ over\ 200\ minutes$

procedure $sort\_ascending(F6Plist, Parameterlist)$
    $Sort\ F6Plist\ in\ ascending\ order\ where\ Parameterlist\ elements\ are\ rearranged\ to\ match\ accordingly$

procedure $minimize(objfunct, p_1, p_2, p_3, p_4)$
    $Perform\ least\ squares\ regression\ using\ LMA\ (ref: http://mathworld.wolfram.com/Levenberg-MarquardtMethod.html)\ using\ 'objfunct'\ as\ the\ objective\ function\ and\ p_1, p_2, p_3, p_4\ as\ initial\ estimation$
