

Supporting material

Solution of a complex nonlinear fractional biochemical reaction model

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Analytical expressions for the concentrations using LDM

The Laplace expressions for the concentrations of enzyme, inhibitor, substrate, product, and the complex intermediate species are derived by solving the nonlinear biochemical reaction system (1) subject to initial conditions given in Eq. (20) and rate constants given in Eq. (21).

For the integer case $\alpha = 1$, the analytical expressions for the concentrations are given by

$$\begin{aligned} E(t) &= 0.1 - 0.0029t + 0.00077805t^2 - 0.000152t^3 + 0.000024t^4 - 0.000003t^5, \\ S(t) &= 0.2 - 0.0011t + 0.000073t^2 - 0.000024t^3 + 0.000004t^4 - 0.0000003t^5, \\ I(t) &= 0.01 - 0.0009t + 0.00014t^2 - 0.000011t^3 - 0.000001t^4 + 0.0000007t^5, \\ P(t) &= 0.0004t^2 - 0.000085t^3 + 0.000014t^4 - 0.000002t^5 + 0.0000003t^6, \\ C_1(t) &= 0.002t - 0.000639t^2 + 0.000141t^3 - 0.000025t^4 + 0.000004t^5, \\ C_2(t) &= 0.0009t - 0.00016155t^2 + 0.000024t^3 - 0.000004t^4 + 0.000001t^5, \\ C_3(t) &= 0.000022t^2 - 0.000014t^3 + 0.000005t^4 - 0.000002t^5 + 0.000004t^6, \end{aligned} \tag{1}$$

For the fractional case $\alpha = 0.9$, the analytical expressions for the concentrations are given by

$$\begin{aligned} E(t) &= 0.1 - 0.003015t^{\frac{9}{10}} + 0.000852t^{\frac{19}{10}} - 0.000172t^{\frac{29}{10}} + 0.000028t^{\frac{39}{10}} - 0.000004t^{\frac{49}{10}}, \\ S(t) &= 0.2 - 0.001144t^{\frac{9}{10}} + 0.00008t^{\frac{19}{10}} - 0.000027t^{\frac{29}{10}} + 0.000004t^{\frac{39}{10}} - 0.0000003t^{\frac{49}{10}}, \\ I(t) &= 0.01 - 0.000936t^{\frac{9}{10}} + 0.000153t^{\frac{19}{10}} - 0.000012t^{\frac{29}{10}} - 0.000001t^{\frac{39}{10}} + 0.0000009t^{\frac{49}{10}}, \\ P(t) &= 0.000438t^{\frac{19}{10}} - 0.000096t^{\frac{29}{10}} + 0.000016t^{\frac{39}{10}} - 0.000002t^{\frac{49}{10}} + 0.0000003t^{\frac{59}{10}}, \\ C_1(t) &= 0.00208t^{\frac{9}{10}} - 0.000699t^{\frac{19}{10}} + 0.00016t^{\frac{29}{10}} - 0.000029t^{\frac{39}{10}} + 0.000005t^{\frac{49}{10}}, \\ C_2(t) &= 0.000936t^{\frac{9}{10}} - 0.000177t^{\frac{19}{10}} + 0.000028t^{\frac{29}{10}} - 0.000005t^{\frac{39}{10}} + 0.000001t^{\frac{49}{10}}, \\ C_3(t) &= 0.000024t^{\frac{19}{10}} - 0.000016t^{\frac{29}{10}} + 0.000006t^{\frac{39}{10}} - 0.000002t^{\frac{49}{10}} + 0.000005t^{\frac{59}{10}}, \end{aligned} \tag{2}$$

For the fractional case $\alpha = 0.8$, the analytical expressions for the concentrations are given by

$$\begin{aligned}
E(t) &= 0.1 - 0.003114t^{\frac{4}{5}} + 0.000929t^{\frac{9}{5}} - 0.000194t^{\frac{14}{5}} + 0.000032t^{\frac{19}{5}} - 0.000005t^{\frac{24}{5}}, \\
S(t) &= 0.2 - 0.001181t^{\frac{4}{5}} + 0.000087t^{\frac{9}{5}} - 0.00003t^{\frac{14}{5}} + 0.000005t^{\frac{19}{5}} - 0.0000004t^{\frac{24}{5}}, \\
I(t) &= 0.01 - 0.000966t^{\frac{4}{5}} + 0.000166t^{\frac{9}{5}} - 0.000014t^{\frac{14}{5}} - 0.0000016t^{\frac{19}{5}} + 0.000001t^{\frac{24}{5}}, \\
P(t) &= 0.000477t^{\frac{9}{5}} - 0.000109t^{\frac{14}{5}} + 0.000019t^{\frac{19}{5}} - 0.000003t^{\frac{24}{5}}, \\
C_1(t) &= 0.002147t^{\frac{4}{5}} - 0.000762t^{\frac{9}{5}} + 0.00018t^{\frac{14}{5}} - 0.000034t^{\frac{19}{5}} + 0.000006t^{\frac{24}{5}}, \\
C_2(t) &= 0.000966t^{\frac{4}{5}} - 0.000193t^{\frac{9}{5}} + 0.000031t^{\frac{14}{5}} - 0.000001t^{\frac{19}{5}} + 0.000001t^{\frac{24}{5}}, \\
C_3(t) &= 0.000026t^{\frac{9}{5}} - 0.000017t^{\frac{14}{5}} + 0.000007t^{\frac{19}{5}} - 0.000002t^{\frac{24}{5}} + 0.000001t^{\frac{29}{5}}.
\end{aligned} \tag{3}$$

Analytical expressions for the concentrations using coupled Padé-DTM

The nonlinear system (1), subject to large initial concentrations given in Eq. (23) with rate constants given in Eq. (24) and is solved to derive memory concentration expressions for enzyme, inhibitor, substrate, product, and the complex intermediate species. Due to the assumption of large initial concentrations, both Laplace decomposition and differential transformation analytical expressions diverge for integer and fractional choice of α even over a small time-domain $0 \leq t \leq 1$. The application of Padé approximation was used to overcome the divergence obstacle. The divergent analytical expressions for the case $\alpha = 1$ for the Laplace and differential transformation are below.

$$\begin{aligned}
E(t) &= 12 - 5.16t + 7.28t^2 - 8.503t^3 + 7.735t^4 - 5.475t^5 + 3.421t^6 - 3.2271t^7 + 5.224t^8 \\
&\quad - 8.054t^9 + 9.538t^{10}, \\
S(t) &= 5 + 3.96t - 9.875t^2 + 11.481t^3 - 7.076t^4 - 0.762t^5 + 6.525t^6 - 5.526t^7 - 2.43t^8 \\
&\quad + 12.28t^9 - 16.807t^{10}, \\
I(t) &= 2 - 4.56t + 7.079t^2 - 8.327t^3 + 7.546t^4 - 5.294t^5 + 3.262t^6 - 3.068t^7 + 5.024t^8 \\
&\quad - 7.787t^9 + 9.222t^{10}, \\
P(t) &= 0.012t^2 - 0.003t^3 + 0.002t^4 - 0.002t^5 + 0.001t^6 - 0.001t^7 + 0.001t^8 - 0.001t^9 + 0.001t^{10}, \\
C_1(t) &= 0.60t - 0.203t^2 + 0.176t^3 - 0.189t^4 + 0.180t^5 - 0.159t^6 + 0.159t^7 - 0.2t^8, \\
&\quad + 0.263t^9 - 0.316t^{10}, \\
C_2(t) &= 4.56t - 9.827t^2 + 11.153t^3 - 6.647t^4 - 1.176t^5 + 6.849t^6 - 5.733t^7 - 2.315t^8 \\
&\quad + 12.19t^9 - 16.664t^{10}, \\
C_3(t) &= 2.748t^2 - 2.826t^3 - 0.898t^4 + 6.47t^5 - 10.111t^6 + 8.801t^7 - 2.709t^8 - 4.404t^9 + 7.442t^{10}.
\end{aligned} \tag{4}$$

The convergent Padé-differential transformation analytical expressions are given by

$$\begin{aligned}
E(t)_{[4/4]} &= \frac{12 + 25.52713t + 29.43211t^2 + 14.87748t^3 + 2.04881t^4}{1 + 2.55726t + 2.94545t^2 + 1.66304t^3 + 0.26583t^4}, \\
S(t)_{[4/4]} &= \frac{5 + 26.67512t + 46.74564t^2 + 30.50806t^3 + 7.73589t^4}{1 + 4.54302t + 7.72613t^2 + 6.65909t^3 + 2.51616t^4}, \\
I(t)_{[4/4]} &= \frac{2 + 0.33854t + 1.30662t^2 - 0.47448t^3 + 0.12989t^4}{1 + 2.44927t + 2.69825t^2 + 1.40927t^3 + 0.15249t^4}, \\
P(t)_{[4/4]} &= \frac{0.012t^2 - 0.03157t^3 - 0.0219t^4}{1 - 2.40505t - 2.51483t^2 - 0.0895t^3 - 0.0548t^4}, \\
C_1(t)_{[4/4]} &= \frac{0.6t + 1.30491t^2 + 1.35654t^3 + 0.64222t^4}{1 + 2.51386t + 2.81977t^2 + 1.60421t^3 + 0.20917t^4}, \\
C_2(t)_{[4/4]} &= \frac{4.56t + 2.23591t^2 - 0.47703t^3 + 0.12628t^4}{1 + 2.64533t + 3.15022t^2 + 1.80405t^3 + 0.29694t^4}, \\
C_3(t)_{[4/4]} &= \frac{2.748t^2 + 4.44026t^3 + 0.15634t^4}{1 + 2.64428t + 3.10333t^2 + 1.701552957t^3 + 0.21788t^4}.
\end{aligned} \tag{5}$$

The analytical concentrations for the case $\alpha = 0.9$ are given by

$$\begin{aligned}
E(t) &= 12 - 5.365t^{\frac{9}{10}} + 8.687t^{\frac{9}{5}} - 12.122t^{\frac{27}{10}} + 13.562t^{\frac{18}{5}} - 12.089t^{\frac{9}{2}} + 9.36t^{\frac{27}{5}} - 9.449t^{\frac{63}{10}} \\
&\quad + 16.454t^{\frac{36}{5}} - 30.788t^{\frac{81}{10}} + 46.743t^9 - 54.278t^{\frac{99}{10}}, \\
S(t) &= 5 + 4.117t^{\frac{9}{10}} - 11.781t^{\frac{9}{5}} + 16.567t^{\frac{27}{10}} - 13.457t^{\frac{18}{5}} + \frac{18}{5} + 1.431t^{\frac{9}{2}} + 12.948t^{\frac{27}{5}} - 16.719t^{\frac{63}{10}} \\
&\quad - 1.56t^{\frac{36}{5}} + 40.358t^{\frac{81}{10}} - 78.529t^9 + 82.645t^{\frac{99}{10}}, \\
I(t) &= 2 - 4.741t^{\frac{9}{10}} + 8.445t^{\frac{9}{5}} - 11.909t^{\frac{27}{10}} + 13.314t^{\frac{18}{5}} - 11.82t^{\frac{9}{2}} + 9.0944t^{\frac{27}{5}} - 9.165t^{\frac{63}{10}} \\
&\quad + 16.048t^{\frac{36}{5}} - 30.1138t^{\frac{81}{10}} + 45.7348t^9 - 53.0688t^{\frac{99}{10}}, \\
P(t) &= 0.014t^{\frac{9}{5}} - 0.004t^{\frac{27}{10}} + 0.003t^{\frac{18}{5}} - 0.003t^{\frac{9}{2}} + 0.002t^{\frac{27}{5}} - 0.002t^{\frac{63}{10}} \\
&\quad + 0.002t^{\frac{36}{5}} - 0.002t^{\frac{81}{10}} + 0.004t^9 - 0.005t^{\frac{99}{10}}, \\
C_1(t) &= 0.624t^{\frac{9}{10}} - 0.243t^{\frac{9}{5}} + 0.213t^{\frac{27}{10}} - 0.248t^{\frac{18}{5}} + 0.269t^{\frac{9}{2}} - 0.266t^{\frac{27}{5}} + 0.284t^{\frac{63}{10}} \\
&\quad - 0.406t^{\frac{36}{5}} + 0.675t^{\frac{81}{10}} - 1.009t^9 + 1.21t^{\frac{99}{10}}, \\
C_2(t) &= 4.741t^{\frac{9}{10}} - 11.723t^{\frac{9}{5}} + 16.104t^{\frac{27}{10}} - 12.731t^{\frac{18}{5}} + 0.588t^{\frac{9}{2}} + 13.744t^{\frac{27}{5}} - 17.339t^{\frac{63}{10}} \\
&\quad - 1.126t^{\frac{36}{5}} + 39.941t^{\frac{81}{10}} - 77.787t^9 + 81.177t^{\frac{99}{10}}, \\
C_3(t) &= 3.278t^{\frac{9}{10}} - 4.195t^{\frac{27}{10}} - 0.582t^{\frac{18}{5}} + 11.232t^{9/2} - 22.838t^{27/5} + 26.504t^{\frac{63}{10}} \\
&\quad - 14.922t^{\frac{36}{5}} - 9.828t^{\frac{81}{10}} + 32.053t^9 - 28.109t^{\frac{99}{10}}.
\end{aligned} \tag{6}$$

The analytical concentrations for the case $\alpha = 0.8$ are given below.

$$\begin{aligned}
E(t) &= 2 - 5.540t^{\frac{4}{5}} + 10.188t^{\frac{8}{5}} - 16.823t^{\frac{12}{5}} + 22.94t^{\frac{16}{5}} - 25.562t^4 + 24.674t^{\frac{24}{5}} - 27.54t^{\frac{28}{5}} \\
&\quad + 49.916t^{\frac{32}{5}} - 109.208t^{\frac{36}{5}} + 208.09t^8 - 316.665t^{\frac{44}{5}} + 373.340t^{\frac{48}{5}}, \\
S(t) &= 5 + 4.252t^{\frac{4}{5}} - 13.815t^{\frac{8}{5}} + 23.238t^{\frac{12}{5}} - 24.326t^{\frac{16}{5}} + 8.676t^4 + 22.024t^{\frac{24}{5}} - 44.421t^{\frac{28}{5}} \\
&\quad + 13.026t^{\frac{32}{5}} + 114.435t^{\frac{36}{5}} - 323.344t^8 + 488.764t^{\frac{44}{5}} - 387.889t^{\frac{48}{5}}, \\
I(t) &= 2 - 4.896t^{\frac{4}{5}} + 9.9036t^{\frac{8}{5}} - 16.573t^{\frac{12}{5}} + 22.646t^{\frac{16}{5}} - 25.221t^4 + 24.331t^{\frac{24}{5}} - 27.211t^{\frac{28}{5}} \\
&\quad + 49.437t^{\frac{32}{5}} - 108.157t^{\frac{36}{5}} + 206.002t^8 - 313.687t^{\frac{44}{5}} + 371.055t^{\frac{48}{5}}, \\
I(t) &= 2 - 4.896t^{\frac{4}{5}} + 9.9036t^{\frac{8}{5}} - 16.573t^{\frac{12}{5}} + 22.646t^{\frac{16}{5}} - 25.221t^4 + 24.331t^{\frac{24}{5}} - 27.211t^{\frac{28}{5}} \\
&\quad + 49.437t^{\frac{32}{5}} - 108.157t^{\frac{36}{5}} + 206.002t^8 - 313.687t^{\frac{44}{5}} + 371.055t^{\frac{48}{5}}, \\
P(t) &= 0.017t^{\frac{8}{5}} - 0.005t^{\frac{12}{5}} + 0.004t^{\frac{16}{5}} - 0.004t^4 + 0.004t^{\frac{24}{5}} - 0.003t^{\frac{28}{5}} \\
&\quad + 0.003t^{\frac{32}{5}} - 0.004t^{\frac{36}{5}} + 0.008t^8 - 0.015t^{\frac{44}{5}} + 0.019t^{\frac{48}{5}}, \\
C_1(t) &= 0.644t^{\frac{4}{5}} - 0.285t^{\frac{8}{5}} + 0.249t^{\frac{12}{5}} - 0.294t^{\frac{16}{5}} + 0.34t^4 - 0.343t^{\frac{24}{5}} + 0.33t^{\frac{28}{5}} - 0.479t^{\frac{32}{5}} \\
&\quad + 1.051t^{\frac{36}{5}} - 2.088t^8 + 2.977t^{\frac{44}{5}} - 2.285t^{\frac{48}{5}}, \\
C_2(t) &= 4.896t^{\frac{4}{5}} - 13.747t^{\frac{8}{5}} + 22.601t^{\frac{12}{5}} - 23.136t^{\frac{16}{5}} + 7.02t^4 + 23.905t^{\frac{24}{5}} - 46.205t^{\frac{28}{5}} + 14.567t^{\frac{32}{5}} \\
&\quad + 112.662t^{\frac{36}{5}} - 319.784t^8 + 480.654t^{\frac{44}{5}} - 371.95t^{\frac{48}{5}}, \\
C_3(t) &= 3.844t^{\frac{8}{5}} - 6.028t^{\frac{12}{5}} + 0.49t^{\frac{16}{5}} + 18.201t^4 - 48.236t^{\frac{24}{5}} + 73.415t^{\frac{28}{5}} - 64.005t^{\frac{32}{5}} - 4.505t^{\frac{36}{5}} \\
&\quad + 113.782t^8 - 166.967t^{\frac{44}{5}} + 0.895t^{\frac{48}{5}}.
\end{aligned} \tag{7}$$

Large order of Padé approximation was required to obtain convergent expressions for the cases $\alpha = 0.9$ and $\alpha = 0.8$.