Effective Reaction Rates for Reaction Sequences - 12Aug2017

In this note we show how reaction sequences may, under steady state assumptions, be replaced with a simpler reaction sequence and effective rate. These techniques are widely used in hardwired approximation reaction networks. The aim is to reduce the number of isotopes evolved in a reaction network, and thus the execution time of an implicit integration. The cost is a more complicated Jacobian matrix as the effective reaction rates depend on the abundances.

1. (a,p)(p,g) sequences

Consider the reaction sequence I(a,p)L(p,g)O

I(a,p)L(p,g)O

f1 $\longrightarrow$ f2 $\longrightarrow$

$\longleftarrow$ r1 $\longleftarrow$ r2

I(a,g)O

f3 $\longrightarrow$

$\longleftarrow$ r3

where I(a,p)L occurrs in the forward direction with a reaction rate f_1 and a reverse reaction rate r_1. Similarly, L(p,g)O occurs in the forward direction with a reaction rate f_2 and a reverse reaction rate r_2. The goal is to reduce the sequence I(a,p)L(p,g)O to the sequence I(a,g)O with an effective forward, f_3, and effective reverse, r_3, reaction rate such the that species L does not need to be included in the reaction network.

Writing out all the terms associated with the full reaction sequence

$$\dot{Y}(I) = -Y(I)\, Y(a)\, f_1 + Y(p)\, Y(L)\, r_1 \tag{1}$$

$$\dot{Y}(a) = -Y(I)\, Y(a)\, f_1 + Y(p)\, Y(L)\, r_1 \tag{2}$$

$$\dot{Y}(p) = +Y(I)\, Y(a)\, f_1 - Y(p)\, Y(L)\, r_1 - Y(L)\, Y(p)\, f_2 + Y(O)\, r_2 \tag{3}$$

$$\dot{Y}(L) = +Y(I)\, Y(a)\, f_1 - Y(p)\, Y(L)\, r_1 - Y(L)\, Y(p)\, f_2 + Y(O)\, r_2 \tag{4}$$

$$\dot{Y}(O) = +Y(L)\, Y(p)\, f_2 - Y(O)\, r_2\ . \tag{5}$$

Assume $\dot{Y}(L) = 0$ so that the abundance of $Y(L)$ is in steady state. In this specific case, $\dot{Y}(L) = 0$ also means $\dot{Y}(p) = 0$, the an explicit proton abundance does not need to be evolved either. Rearranging Eq. 4,

$$Y(I)\, Y(a)\, f_1 + Y(O)\, r_2 = Y(p)\, Y(L)\, r_1 + Y(L)\, Y(p)\, f_2\ \ . \tag{6}$$

Solving for $Y(p)Y(L)$

$$Y(p)Y(L) = \frac{Y(I)\ Y(a)\ f_1 + Y(O)\ r_2}{r_1 + f_2}\ . \tag{7}$$

Let

$$v = \frac{r_1}{r_1 + f_2}\ . \tag{8}$$

Note that

$$\frac{r_1}{r_1 + f_2} + \frac{f_2}{r_1 + f_2} = 1 \tag{9}$$

or

$$\frac{f_2}{r_1 + f_2} = 1 - v\ \ . \tag{10}$$

Substituting Eq. 7 and Eq. 8 into Eq. (1)

$$\begin{aligned}
\dot{Y}(I) &= -Y(I)\ Y(a)\ f_1 + Y(p)\ Y(L)\ r_1 \\
&= -Y(I)\ Y(a)\ f_1 + \left[\frac{Y(I)\ Y(a)\ f_1 + Y(O)\ r_2}{r_1 + f_2}\right]\ r_1 \\
&= -Y(I)\ Y(a)\ f_1 + [Y(I)\ Y(a)\ f_1 + Y(O)\ r_2]\ v \\
&= -Y(I)\ Y(a)\ f_1\ (1 - v) + Y(O)\ r_2\ v\ .
\end{aligned} \tag{11}$$

This identifies the effective reaction rates f_3 and r_3 as

$$\begin{aligned}
f_3 &= f_1\ (1 - v) = \frac{f_1 \cdot f_2}{r_1 + f_2} \\
r_3 &= r_2\ v = \frac{r_1 \cdot r_2}{r_1 + f_2}\ ,
\end{aligned} \tag{12}$$

and we have the desired final form

$$\dot{Y}(I) = -Y(I)\ Y(a)\ f_3 + Y(O)\ f_3\ . \tag{13}$$

Since the ODE for Y(a) is identical to that for Y(I),

$$\dot{Y}(a) = -Y(I)\ Y(a)\ f_3 + Y(O)\ r_3\ . \tag{14}$$

Substituting Eq. 7 and Eq. 10 into Eq. (5)

$$\begin{aligned}
\dot{Y}(O) &= Y(L)\ Y(p)\ f_2 - Y(O)\ r_2 \\
&= \left[\frac{Y(I)\ Y(a)\ f_1 + Y(O)\ r_2}{r_1 + f_2}\right]\ f_2 - Y(O)\ r_2 \\
&= [Y(I)\ Y(a)\ f_1 + Y(O)\ r_2]\ (1 - v) - Y(O)\ r_2 \\
&= Y(I)\ Y(a)\ f_1(1 - v) - Y(O)\ r_2\ v \\
&= Y(I)\ Y(a)\ f_3 - Y(O)\ r_3\ .
\end{aligned} \tag{15}$$

Equations 13, 14, and 15 constitute the simpler sequence I(a,g)O with a effective forward, f_3, and an effective reverse, r_3, reaction rate such the that species L or p does not need to be included in the reaction network.

Some limits. Note that $v \rightarrow 0$ when $f_2 >> r_1$. This means the (p,g) reaction rate is much stronger than the (p,a) reaction rate, allowing flows to species O. The ODEs reduce to

$$\begin{aligned} \dot{Y}(I) &= -Y(I)\ Y(a)\ f_1 \\ \dot{Y}(a) &= -Y(I)\ Y(a)\ f_1 \\ \dot{Y}(O) &= +Y(I)\ Y(a)\ f_1 \end{aligned} \tag{16}$$

as expected. Similarily, $v \rightarrow 1$ when $r_1 >> f_2$, meaning the (p,a) reaction rate is much stronger than the (p,g) reaction rate and thus inhibiting flows to species O. The ODEs reduce to

$$\begin{aligned} \dot{Y}(I) &= +Y(O)\ r_2 \\ \dot{Y}(a) &= +Y(O)\ r_2 \\ \dot{Y}(O) &= -Y(O)\ r_2 \end{aligned} \tag{17}$$

as expected.

Similar expressions hold for (a,n)(n,g) sequences with the obvious replacement of Y(n) for Y(p) in equations 13, 14, and 15.

2. (n,g)(n,g) sequences

Consider the reaction sequence I(n,g)L(n,g)O

$$\mathrm{I(n,g)L(n,g)O}$$
$$\begin{array}{cc} \mathrm{f1}\longrightarrow & \mathrm{f2}\longrightarrow \\ \longleftarrow\mathrm{r1} & \longleftarrow\mathrm{r2} \end{array}$$

$$\mathrm{I(2n,2g)O}$$
$$\begin{array}{c} \mathrm{f3}\longrightarrow \\ \longleftarrow\mathrm{r3} \end{array}$$

As above, the goal is to reduce the sequence I(n,g)L(n,g)O to the simpler sequence I(2n,2g)O with an effective forward rate f_3 and an effective reverse rate r_3 such the that species L does not need to be included in the reaction network.

Writing out all the terms associated with the full reaction sequence

$$\dot{Y}(I) = -Y(I)\,Y(n)\,f_1 + Y(L)\,r_1 \tag{18}$$
$$\dot{Y}(n) = -Y(I)\,Y(n)\,f_1 + Y(L)\,r_1 - Y(L)\,Y(n)\,f_2 + Y(O)\,r_2 \tag{19}$$
$$\dot{Y}(L) = +Y(I)\,Y(n)\,f_1 - Y(L)\,r_1 - Y(L)\,Y(n)\,f_2 + Y(O)\,r_2 \tag{20}$$
$$\dot{Y}(O) = +Y(L)\,Y(n)\,f_2 - Y(O)\,r_2 \;\; . \tag{21}$$

Assume $\dot{Y}(L) = 0$ so that the abundance of $Y(L)$ is in steady state. Rearranging Eq. 20,

$$Y(L)\,Y(n)\,f_2 + Y(L)\,r_1 = Y(I)\,Y(n)\,f_1 + Y(O)\,r_2 \; . \tag{22}$$

Solving for $Y(L)$

$$Y(L) = \frac{Y(I)\,Y(n)\,f_1 + Y(O)\,r_2}{r_1 + Y(n)\,f_2} \; . \tag{23}$$

Let

$$v = \frac{r_1}{r_1 + Y(n)\,f_2} \; , \tag{24}$$

which implies

$$\frac{r_1}{r_1 + Y(n)\,f_2} + \frac{Y(n)\,f_2}{r_1 + Y(n)\,f_2} = 1 \tag{25}$$

or

$$\frac{Y(n)\,f_2}{r_1 + Y(n)\,f_2} = 1 - v \; . \tag{26}$$

Substituting Eq. 23 and Eq. 24 into Eq. (18)

$$\begin{aligned}\dot{Y}(I) &= -Y(I)\,Y(n)\,f_1 + Y(L)\,r_1 \\ &= -Y(I)\,Y(n)\,f_1 + \left[\frac{Y(I)\,Y(n)\,f_1 + Y(O)\,r_2}{r_1 + Y(n)\,f_2}\right] r_1 \\ &= -Y(I)\,Y(n)\,f_1 + [Y(I)\,Y(n)\,f_1 + Y(O)\,r_2]\,v \\ &= -Y(I)\,Y(n)\,f_1\,(1-v) + Y(O)\,r_2\,v\,. \end{aligned} \tag{27}$$

This identifies the effective reaction rates f_3 and r_3 as

$$\begin{aligned} f_3 &= f_1\,(1-v) = \frac{f_1 \cdot Y(n)\,f_2}{r_1 + Y(n)\,f_2} \\ r_3 &= r_2\,v = \frac{r_1 \cdot r_2}{r_1 + Y(n)\,f_2}\,, \end{aligned} \tag{28}$$

and we have the desired final form

$$\dot{Y}(I) = -Y(I)\,Y(n)\,f_3 + Y(O)\,r_3\,. \tag{29}$$

Similarly for Eq (21),

$$\begin{aligned}\dot{Y}(O) &= Y(L)\,Y(n)\,f_2 - Y(O)\,r_2 \\ &= \left[\frac{Y(I)\,Y(n)\,f_1 + Y(O)\,r_2}{r_1 + Y(n)\,f_2}\right] Y(n)\,f_2 - Y(O)\,r_2 \\ &= [Y(I)\,Y(n)\,f_1 + Y(O)\,r_2]\,(1-v) - Y(O)\,r_2 \\ &= Y(I)\,Y(n)\,f_1(1-v) - Y(O)\,r_2\,v \\ &= Y(I)\,Y(n)\,f_3 - Y(O)\,r_3\,. \end{aligned} \tag{30}$$

And for the neutron abundance of Eq. (19),

$$\begin{aligned}\dot{Y}(n) &= -Y(I)\,Y(n)\,f_1 + Y(L)\,r_1 - Y(L)\,Y(n)\,f_2 + Y(O)\,r_2 \\ &= -Y(I)\,Y(n)\,f_1 + \left[\frac{Y(I)\,Y(n)\,f_1 + Y(O)\,r_2}{r_1 + Y(n)\,f_2}\right] r_1 - \left[\frac{Y(I)\,Y(n)\,f_1 + Y(O)\,r_2}{r_1 + Y(n)\,f_2}\right] Y(n)\,f_2 + Y(O)\,r_2 \\ &= -Y(I)\,Y(n)\,f_1 + [Y(I)\,Y(n)\,f_1 + Y(O)\,r_2]\,v - [Y(I)\,Y(n)\,f_1 + Y(O)\,r_2]\,(1-v) - Y(O)\,r_2 \\ &= -2\,Y(I)\,Y(n)\,f_2\,(1-v) + 2Y(O)\,r_2\,v \\ &= -2\,Y(I)\,Y(n)\,f_3 + 2Y(O)\,r_3\,. \end{aligned} \tag{31}$$

Equations 29, 30, and 31 constitute the simpler sequence I(2n,2g)O with a effective forward rate, f_3, and an effective reverse rate, r_3, such the that species L does not need to be included in the reaction network.

Similar expressions hold for (p,g)(p,g) sequences with the obvious replacement of Y(p) for Y(n) in equations 29, 30, and 31.

3. (a,p)(g,p) sequences

Consider the reaction sequence I(a,p)L(g,p)O, which has less symmetry than the previous two cases. As before, the goal is to reduce this sequence to the simpler sequence I(a,2p)O with an effective forward, f_3, and effective reverse, r_3, reaction rate such the that species L does not need to be included in the reaction network.

Writing out all the terms associated with the full reaction sequence

$$\dot{Y}(I) = -Y(I)\, Y(a)\, f_1 + Y(L)\, Y(p)\, r_1 \tag{32}$$
$$\dot{Y}(a) = -Y(I)\, Y(a)\, f_1 + Y(L)\, Y(p)\, r_1 \tag{33}$$
$$\dot{Y}(p) = +Y(I)\, Y(a)\, f_1 - Y(L)\, Y(p)\, r_1 + Y(L)\, f_2 - Y(O)\, Y(p)\, r_2 \tag{34}$$
$$\dot{Y}(L) = +Y(I)\, Y(a)\, f_1 - Y(L)\, Y(p)\, r_1 - Y(L)\, f_2 + Y(O)\, Y(p)\, r_2 \tag{35}$$
$$\dot{Y}(O) = +Y(L)\, f_2 - Y(O)\, Y(p)\, r_2\ . \tag{36}$$

Assuming $\dot{Y}(L) = 0$ so that $Y(L)$ is in steady state. Rearranging Eq. 35,

$$Y(I)\, Y(a)\, f_1 + Y(O)\, Y(p)\, r_2 = Y(L)\, Y(p)\, r_1 + Y(L)\, f_2\ . \tag{37}$$

Solving for $Y(L)$

$$Y(L) = \frac{Y(I)\, Y(a)\, f_1 + Y(O)\, Y(p)\, r_2}{f_2 + Y(p)\, r_1}\ . \tag{38}$$

Let

$$v = \frac{Y(p)\, r_1}{f_2 + Y(p)\, r_1}\ . \tag{39}$$

This definition implies

$$\frac{Y(p)\, r_1}{f_2 + Y(p)\, r_1} + \frac{f_2}{f_2 + Y(p)\, r_1} = 1 \tag{40}$$

or

$$\frac{f_2}{f_2 + Y(p)\, r_1} = 1 - v\ . \tag{41}$$

Substituting Eq. 38 and Eq. 39 into Eq. (32)

$$\begin{aligned} \dot{Y}(I) &= -Y(I)\, Y(a)\, f_1 + Y(L)\, Y(p)\, r_1 \\ &= -Y(I)\, Y(a)\, f_1 + \left[\frac{Y(I)\, Y(a)\, f_1 + Y(O)\, Y(p)\, r_2}{f_2 + Y(p)\, r_1}\right] r_1 \\ &= -Y(I)\, Y(a)\, f_1 + [Y(I)\, Y(a)\, f_1 + Y(O)\, Y(p)\, r_2]\, v \\ &= -Y(I)\, Y(a)\, f_1\, (1 - v) + Y(O)\, Y(p)\, r_2\, v\ . \end{aligned} \tag{42}$$

This identifies the effective reaction rates f_3 and r_3 as

$$\begin{aligned} f_3 &= f_1\, (1 - v) = \frac{f_1 f_2}{f_2 + Y(p)\, r_1} \\ r_3 &= r_2\, v = \frac{Y(p)\, r_1\, r_2}{f_2 + Y(p)\, r_1}\ , \end{aligned} \tag{43}$$

and we have the desired final forms

$$\dot{Y}(I) = -Y(I)\,Y(a)\,f_3 + Y(O)\,Y(p)\,r_3 \tag{44}$$

$$\dot{Y}(a) = -Y(I)\,Y(a)\,f_3 + Y(O)\,Y(p)\,r_3 \tag{45}$$

$$\dot{Y}(O) = Y(I)\,Y(a)\,f_3 - Y(O)\,Y(p)\,r_3 \tag{46}$$

$$\dot{Y}(p) = 2\,Y(I)\,Y(a)\,f_3 - 2Y(O)\,Y(p)\,r_3\ . \tag{47}$$

which constitute the simpler sequence I(a,2p)O with a effective forward, f_3, and an effective reverse, r_3, reaction rate such the that species L does not need to be included in the reaction network.

Similar expressions hold for (a,n)(g,n) sequences with the obvious replacement of Y(n) for Y(p).