

(*
equation17.nb

produced by D.F.Gochberg for paper:
D.F.Gochberg, M.D.Does, Z.Zu, C.L.Lankford. Towards
an analytic solution for pulsed CEST.NMR in Biomedicine 2017

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Based on: analytic_CEST_zb_ss and lab notebook 27,
p.29 (Dan's reminder to himself)
*)

(* equivalent formulations of steady state: *)

(* form used in some matlab calculations: *)

$$ss = \text{Inverse} \left[\begin{pmatrix} r2b + kba & -dwb & 0 \\ dwb & r2b + kba & -w1 \\ 0 & w1 & r1b + kba \end{pmatrix} \right] \cdot \begin{pmatrix} kba * r1a * dwa * w1 / (R1rho * (w1^2 + dwa^2)) \\ 0 \\ kba * dwa^2 * r1a / (R1rho * (w1^2 + dwa^2)) + r1b \end{pmatrix};$$

(* form used to derive eqn 17: *)

$$ss3 = \text{Inverse} \left[\begin{pmatrix} r2b + kba & -dwb & 0 \\ dwb & r2b + kba & -w1 \\ 0 & w1 & r1b + kba \end{pmatrix} \right] \cdot \begin{pmatrix} kba * zaSS * w1 / dwa \\ 0 \\ kba * zaSS + r1b \end{pmatrix};$$

(* The ratio between zaSS and xaSS is sinA/cosA = w1a/dwa *)

(* equation 17 comes from combining the 2 numerator and denominator terms: *)

```
ss3Zb = Collect[Simplify[ss3[[3, 1]]], {zaSS}]
```

```
ss3ZbTerm1Num = Collect[Numerator[ss3Zb[[1]]], r1b, Simplify]
```

```
ss3ZbTerm1Den = Collect[Denominator[ss3Zb[[1]]], w1, Simplify]
```

```
ss3ZbTerm2Num = Collect[Numerator[ss3Zb[[2]]] / dwa, zaSS, Simplify]
```

```
ss3ZbTerm2Den = Collect[Denominator[ss3Zb[[2]]] / dwa, w1, Simplify]
```

$$\frac{r1b (dwb^2 + (kba + r2b)^2)}{dwb^2 (kba + r1b) + (kba + r2b) (kba^2 + r1b r2b + kba (r1b + r2b) + w1^2)} + \frac{(dwa kba (dwb^2 + (kba + r2b)^2) + dwb kba w1^2) zaSS}{dwa (dwb^2 (kba + r1b) + (kba + r2b) (kba^2 + r1b r2b + kba (r1b + r2b) + w1^2))}$$

$$r1b (dwb^2 + (kba + r2b)^2)$$

$$(kba + r1b) (dwb^2 + (kba + r2b)^2) + (kba + r2b) w1^2$$

$$kba \left(dwb^2 + (kba + r2b)^2 + \frac{dwb w1^2}{dwa} \right) zaSS$$

$$(kba + r1b) (dwb^2 + (kba + r2b)^2) + (kba + r2b) w1^2$$

(* unitless form of Zb steady state value is

used to derive eqn 28 in equations3and4and28.nb *)

```
normTransforms = {
```

```
  r1b → alpha * w1,
```

```
  r2b → beta * w1,
```

```
  kba → k * w1,
```

```
  dwb → delta * w1,
```

```
  dwa → deltaA * w1
```

```
};
```

```
ss3ZbNorm = Simplify[ss3Zb //. normTransforms]
```

$$\frac{(\alpha \delta A (\beta^2 + \delta^2 + 2 \beta k + k^2) + k (\delta + \delta^2 \delta A + \delta A (\beta + k)^2) zaSS)}{(\delta A (\beta^2 (\alpha + k) + \alpha (\delta^2 + k^2) + k (1 + \delta^2 + k^2) + \beta (1 + 2 \alpha k + 2 k^2)))}$$