

# Reactive Transport Results: Q=1

## example, More

## DOC

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### Predefine some things

```
In[354]:= fstyle = { {Thick, Black, Larger}, {Thick, Black, Larger},  
    {Thick, Black, Larger}, {Thick, Black, Larger}};  
Off[NIntegrate::inumr];  
  
In[356]:= fname = NotebookDirectory[] <> "ADELS-RT.nb";  
NotebookEvaluate[fname];  
Definition[ForwardSolutionRT];  
  
In[359]:= fname = NotebookDirectory[] <> "TSM-RT.nb";  
NotebookEvaluate[fname];  
Definition[ForwardSolutionRTSM];
```

### Channel parameters

```
In[362]:= Q = 1;  
v0 = 0.9 Q^0.35;  
d = 0.4 * Q^0.4;  
w = Q / (v0 d);  
A = w d;  
{A, w, d, v0}  
  
Out[367]= {1.11111, 2.77778, 0.4, 0.9}
```

### biokinetic parameters

Monod parameters are based on Gu et al. 2007. The rate constants kaer and kden were adjusted to get characteristic time scale for O<sub>2</sub> and NO<sub>3</sub> removal to be 1-2 hours, and 5 hours, respectively.

```
In[368]:= kaer = 2 × 10^-3;
kden = 4 × 10^-4;
KaDOC = 45;
KdDOC = 45;
K02 = 6;
K02inh = 0.3;
KN03 = 50;
Fog = 1;
Fng = 0.8;
Caermax = 50;
Cdenmax = 50;
(* side effect for later use *)
kfo = (kden * Fng * Cdenmax) / 130.;

CDOCin = 750.;
CO2in = 250.;
CN03in = 130;
```

## Reference Case; 1 hour median travel time, qnexss=10^-4

Define travel time distribution and rate constant distribution

```
In[383]:= tmean = 5.182 / 2.; (* chosen to make tmedian 1 hours *)
asig = 1;
amean = 1. / tmean;
numsamp = 50;
weight = Table[1./numsamp, {numsamp}];

ldist = LogNormalDistribution[Log[amean] - asig^2/2, asig];
alphasamp = Quantile[ldist, (Range[numsamp] - 0.5) / numsamp] / 3600.;

Clear[t];
hadist = Table[
  foo = t /.
    FindRoot[ 1./amean NIntegrate[ PDF[ldist][alpha] alpha * (1 - Exp[-alpha t]), {alpha, 0.0, 30.}] == q, {t, 0.01, 0, 100}],
  {foo, q}, {q, 0.5/numsamp, 1 - 0.5/numsamp, 1/numsamp}];

tsamp = Transpose[hadist][[1]] * 3600.;
tsamp = Prepend[tsamp, 0.];
Tmedian = t /.
  FindRoot[ 1./amean NIntegrate[ PDF[ldist][alpha] alpha * (1 - Exp[-alpha t]), {alpha, 0.0, 30.}] == 0.5, {t, 0.01, 0, 100}];
Tmedian = Tmedian * 3600.;
```

```
In[396]:= Tmedian / 3600.
Out[396]= 1.00018

In[397]:= Apply[Plus, tsamp] / Length[tsamp] / 3600.
Out[397]= 2.41974

define q for ADELS and volfrac for mTSM

In[398]:= qnexss = 10^-4; (* m/s *)
q = qnexss / d (* 1/s *)
volfrac = q / Apply[Plus, alphasamp] * numsamp
Out[399]= 0.00025

Out[400]= 2.38733
```

## LS model

```
In[401]:= nchansegs = 50;
foo =
ForwardSolutionRT[tsamp, weight, q, 2, nchansegs, {w*d, v0, 3000/nchansegs}];

In[403]:= num = numsamp * nchansegs + nchansegs + 1;
D0Result = Take[foo, num];
foo = Drop[foo, num];
O2result = Take[foo, num];
foo = Drop[foo, num];
N03result = Take[foo, num];
```

## NO3

```
In[409]:= foo = Table[{(i - 0.5) * 3000 / nchansegs,
100 * (1 - N03result[[i]][24 * 3600 * 30] / CN03in)], {i, 1, nchansegs}];
gN03 = ListPlot[foo, PlotRange -> All, Joined -> True, PlotStyle -> {Green, Thick}];
fig6resultN03adels =
Table[100 * (1 - N03result[[i]][24 * 3600 * 30] / CN03in), {i, 1, nchansegs}];
(* analytical solution for comparision *)
gamma = 0.5 q * w d xx / Q;

firstorder =
(1 - gamma * (1 - Exp[-Tmedian * kfo])) / (1 + gamma * (1 - Exp[-Tmedian * kfo]));
g1st = Plot[100 (1 - firstorder), {xx, 0, 3000}];

Removal efficiency at 1000 and 3000 m
```

```
In[415]:= {100 * (1 - N03result[[16]][24 * 3600 * 30] / CN03in) ,
100 * (1 - N03result[[50]][24 * 3600 * 30] / CN03in) }

Out[415]= {6.64275, 19.456}
```

## Subgrid at 1500 m

```
In[416]:= foo = Table[ O2result[[i]][60 * 3600 * 24],
{i, Length[D0Cresult] - 25 * numsamp + 1, Length[D0Cresult] - 24 * numsamp}];
foo = Prepend[foo, O2result[[nchansegs - 24]][60 * 3600 * 24]];
O2adels = foo;
foo = Transpose[{tsamp / (3600), foo}];
g02 = ListLogPlot[foo, Joined → True, PlotStyle → {Blue, Thick}];
foo = Table[N03result[[i]][60 * 3600 * 24],
{i, Length[D0Cresult] - 25 * numsamp + 1, Length[D0Cresult] - 24 * numsamp}];
foo = Prepend[foo, N03result[[nchansegs - 24]][60 * 3600 * 24]];
N03adels = foo;
foo = Transpose[{tsamp / (3600), foo}];
gN03r = ListLogPlot[foo, Joined → True,
PlotRange → {{0, 20}, All}, PlotStyle → {Green, Thick}];
foo = Table[D0Cresult[[i]][60 * 3600 * 24],
{i, Length[D0Cresult] - 25 * numsamp + 1, Length[D0Cresult] - 24 * numsamp}];
foo = Prepend[foo, D0Cresult[[nchansegs - 24]][60 * 3600 * 24]];
D0Cadels = foo;
foo = Transpose[{tsamp / (3600), foo}];

gD0Cr = ListLogPlot[foo, Joined → True,
PlotRange → {{0, 20}, All}, PlotStyle → {Black, Thick}];
```

## Multiple TSMs

```
In[431]:= nchansegs = 50;
foo = ForwardSolutionRTSM[Reverse[alphasamp],
weight, volfrac, 2, nchansegs, {w*d, v0, 3000/nchansegs}];
```

```
In[433]:= num = numsamp * nchansegs + nchansegs + 1;
D0Cresult = Take[foo, num];
foo = Drop[foo, num];
O2result = Take[foo, num];
foo = Drop[foo, num];
N03result = Take[foo, num];
```

## NO3

```
In[439]:= foo = Table[{(i - 0.5) * 3000 / nchansegs,
100 * (1 - N03result[[i]][24 * 3600 * 30] / CN03in )}, {i, 1, nchansegs}];
gN03tsm = ListPlot[foo, PlotRange → All, Joined → True,
PlotStyle → {Green, Thick, Dashed}];
fig6resultN03tsm = Table[100 * (1 - N03result[[i]][24 * 3600 * 30] / CN03in ),
{i, 1, nchansegs}];

(* analytical solution for comparision *)
gamma = 0.5 q * w d xx / Q;
```

Removal efficiency at 1000 and 3000 m

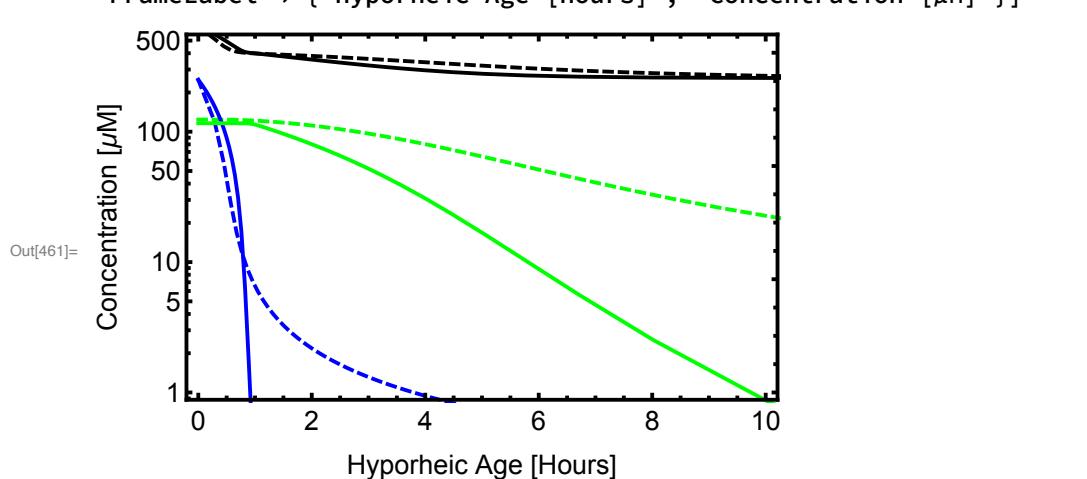
```
In[443]:= {100 * (1 - N03result[[16]][24 * 3600 * 30] / CN03in ),
100 * (1 - N03result[[50]][24 * 3600 * 30] / CN03in )}
Out[443]= {2.88683, 8.60846}
```

## Compare

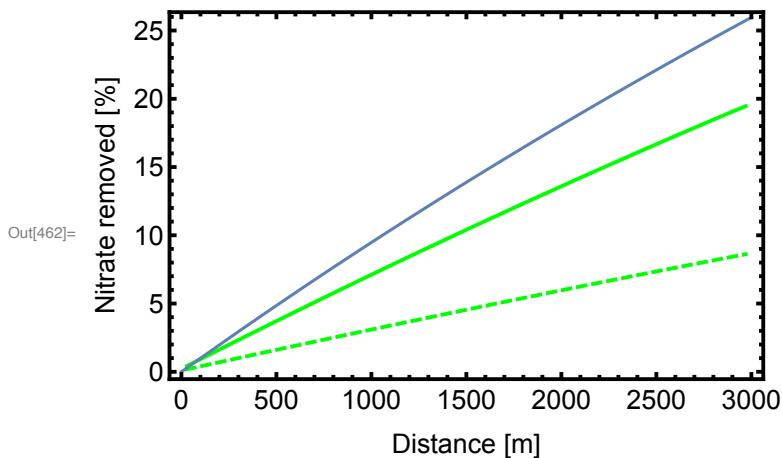
```
In[444]:= tchar = Log[2.] / Reverse[alphasamp];
tchar = Prepend[tchar, 0];
```

```
In[446]:= foo = Table[02result[[i]][60 * 3600 * 24],
  {i, Length[D0Cresult] - 25 * numsamp + 1, Length[D0Cresult] - 24 * numsamp}];
foo = Prepend[foo, 02result[[nchansegs - 24]][60 * 3600 * 24]];
02tsm = foo;
foo = Transpose[{tchar / (3600), foo}];
g021 = ListLogPlot[foo, Joined → True,
  PlotRange → All, PlotStyle → {Blue, Thick, Dashed}];
foo = Table[N03result[[i]][60 * 3600 * 24],
  {i, Length[D0Cresult] - 25 * numsamp + 1, Length[D0Cresult] - 24 * numsamp}];
foo = Prepend[foo, N03result[[nchansegs - 24]][60 * 3600 * 24]];
N03tsm = foo;
foo = Transpose[{tchar / (3600), foo}];
gN031 = ListLogPlot[foo, Joined → True,
  PlotRange → {{0, 10}, All}, PlotStyle → {Green, Thick, Dashed}];
foo = Table[D0Cresult[[i]][60 * 3600 * 24],
  {i, Length[D0Cresult] - 25 * numsamp + 1, Length[D0Cresult] - 24 * numsamp}];
foo = Prepend[foo, D0Cresult[[nchansegs - 24]][60 * 3600 * 24]];
D0Ctsm = foo;
foo = Transpose[{tchar / (3600), foo}];
gD0C1 = ListLogPlot[foo, Joined → True,
  PlotRange → {{0, 10}, All}, PlotStyle → {Black, Thick, Dashed}];

Show[g021, gN031, gD0C1, g02, gN03r, gDOCr, Frame → True,
  FrameStyle → fstyle, PlotRange → {{0, 10}, {0, 6.}}, Axes → False,
  FrameLabel → {"Hyporheic Age [Hours]", "Concentration [\u00b5M]"}]
```



```
In[462]:= Show[gN03, gN03tsm, g1st, Frame → True,
PlotRange → {{0, 3000}, {0, 25}}, Axes → False, FrameStyle → fstyle,
FrameLabel → {"Distance [m]", "Nitrate removed [%]"}]
```



```
In[471]:= fig7resultTSM = Transpose[{tchar / (3600), O2tsm, N03tsm, DOCtsm}];
Export[ "/Users/scottpainter/Dropbox (Personal)/Figure7resultTSM.csv",
fig7resultTSM, "TableHeadings" → {"characteristic time",
"conc O2 micromolar", "conc N03 micromolar", "conc DOC micromolar"}];

In[473]:= fig7resultADELS = Transpose[{tsamp / (3600), O2adel, N03adel, DOCadel}];
Export[ "/Users/scottpainter/Dropbox (Personal)/Figure7resultADELS.csv",
fig7resultADELS, "TableHeadings" → {"hyporheic age [hr]",
"conc O2 micromolar", "conc N03 micromolar", "conc DOC micromolar"}];

In[475]:= distance = Table[(i - 0.5) * 3000 / nchansegs, {i, 1, nchansegs}];
fig6result = Transpose[{distance, fig6resultN03adel, fig6resultN03tsm}];

In[477]:= Export[ "/Users/scottpainter/Dropbox (Personal)/Figure6result.csv", fig6result,
"TableHeadings" → {"distance [m]", "%N03 removed adels", "%N03 removed TSM"}];
```