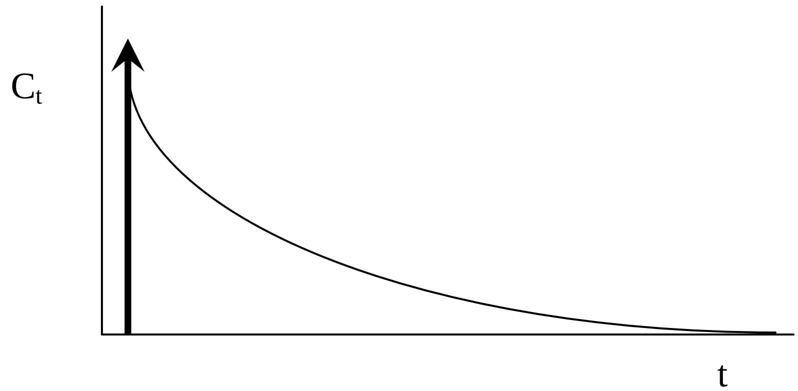
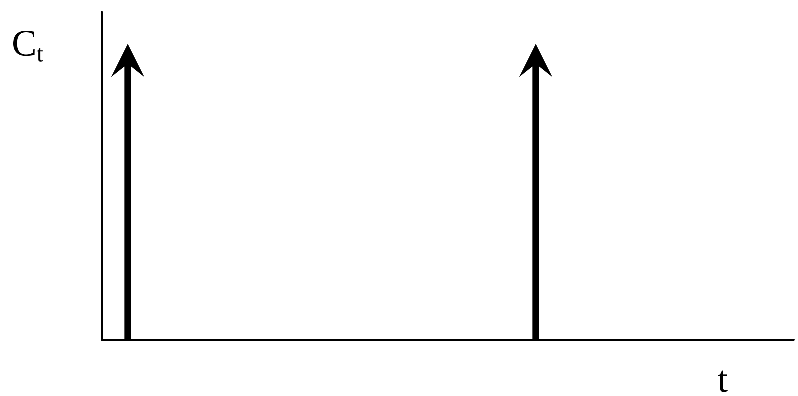
NON-IDEAL REACTORS

Ideal reactor response to pulse tracer:

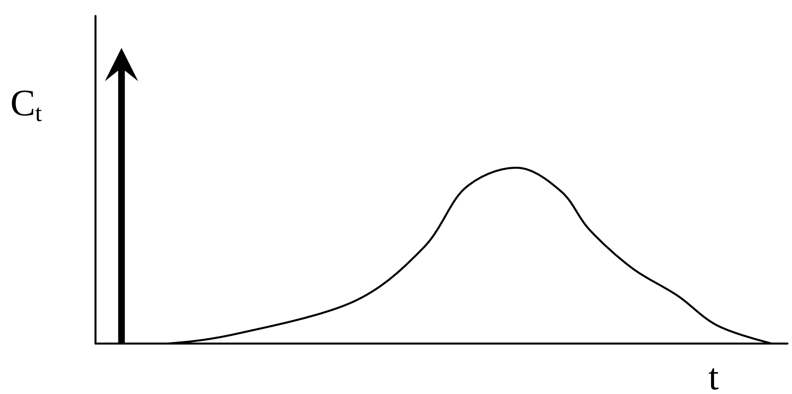
CSTR PULSE RESPONSE



PLUG FLOW REACTOR PULSE RESPONSE



NON-IDEAL REACTOR PULSE RESPONSE



Flow characteristics contributing to non-ideal behavior:

- Short circuiting
- Dead spot
- Non-ideal inlet/outlet conditions
- Diffusion from concentration gradient
- Dispersion from turbulent transport

METHODS OF ANALYSIS TO PREDICT NON-IDEAL REACTOR PERFORMANCE

1. Plug flow with dispersion
2. Residence time distribution (RTD)
3. **Ideal reactor network special case: CSTR cascade**

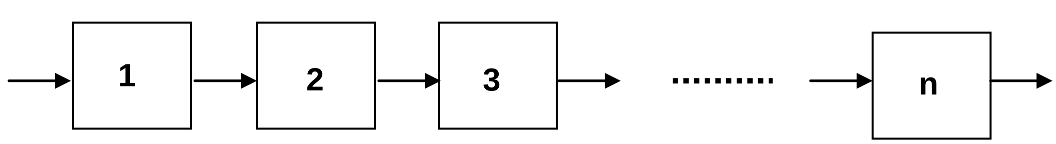
Why is CSTR cascade analysis useful?

Dispersed plug flow ("advection-dispersion") model must be solved numerically for rate models typical of biological reactions.

RTD analysis also requires numerical solutions and is not strictly applicable for non-linear reaction rates (i.e., okay for 1st-order reactions, but not good for zero- or mixed-order)

Advantages of CSTR cascade is enabling mass balance analysis of reactors with complex rate models, flexibility in simulating a variety of mixing (dispersion) conditions, and translates readily into simulation models accommodating multiple coupled reactions.

CSTR Cascade schematic:

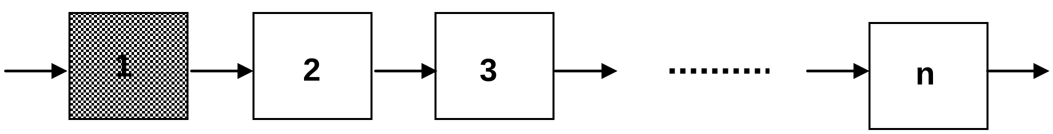


Cascade is comprised of n ideal CSTR's of equal volume in series.

Analysis of response to pulse input of conservative tracer, C, where

V = volume of single CSTR, constant
n = number of CSTR's in cascade
nV = total cascade volume, increases as n increases
Q = volumetric flowrate, constant
τ = single CSTR detention time = V/Q is constant
n τ = cascade total detention time = n(V/Q) increases as n increases
t = time and t/τ = dimensionless time.

Simulate pulse by assuming first tank is filled with tracer, and downstream tanks contain water with no tracer. At t = 0 start clean water influent with no tracer, that is, $C_i(0) = 0$.



Tank 1 mass balance for tracer concentration in influent = $C_i(0) = 0$ and effluent/tank tracer concentration= C_1:

$$\frac{dC_1}{dt} = \frac{C_1}{\tau}$$

Solve for tank boundary conditions $C_t = C_1$ and $C_1(0) = C_O$

$$C_1 = C_O e^{\left(\frac{-t}{\tau}\right)}$$

Tank 2 mass balance:

$$QC_1 = QC_2 + V\frac{dC_2}{dt}$$

$$\frac{dC_2}{dt} + \frac{C_2}{\tau} = \frac{C_O e^{\left(\frac{-t}{\tau}\right)}}{\tau}$$

Solve for boundary conditions $C_t = C_2$ and $C_2(0) = 0$

$$C_2 = \left(\frac{C_O}{\tau}\right) t e^{\left(\frac{-t}{\tau}\right)}$$

Tank 3 mass balance:

$$QC_2 = QC_3 + V\frac{dC_3}{dt}$$

$$\frac{dC_3}{dt} + \frac{C_3}{\tau} = \frac{C_2}{\tau} = \left(\frac{C_O e^{\left(\frac{-t}{\tau}\right)}}{\tau}\right)\left(\frac{1}{\tau}\right) = \left(\frac{C_O e^{\left(\frac{-t}{\tau}\right)}}{\tau^2}\right)$$

Solve for boundary conditions $C_t = C_3$ and $C_3(0) = 0$

$$C_3 = \left(\frac{C_O}{2}\right)\left(\frac{t}{\tau}\right)^2 e^{\left(\frac{-t}{\tau}\right)}$$

Continuing to n^{th} tank…

Tank n mass balance:

$$QC_{n-1} = QC_n + V\frac{dC_n}{dt}$$

Solve for boundary conditions: $C_t = C_n$ and $C_n(0) = 0$

$$C_n = \left(\frac{C_O}{(n-1)!}\right)\left(\frac{t}{\tau}\right)^{(n-1)} e^{\left(\frac{-t}{\tau}\right)}$$

For any tank $n \geq 1$, can get peak effluent/tank tracer concentration and time of peak from:

$$\frac{dC_n}{dt} = 0$$

$$t_{n,peak} = (n-1)\tau$$

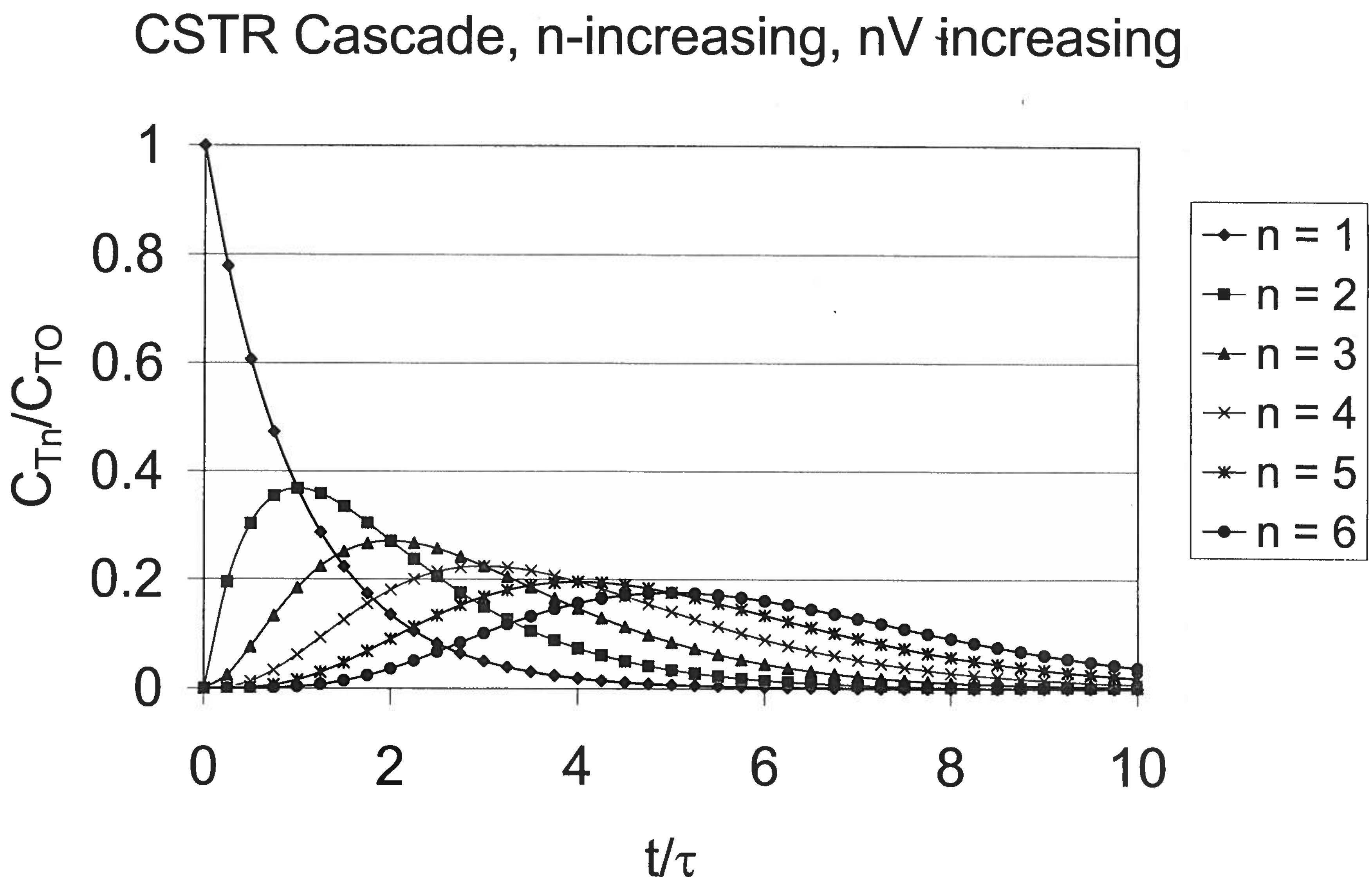
(One-tank CSTR does not have true "peak" but does have maximum at t = 0

And

$$C_{n,peak} = \frac{C_O}{(n-1)!}(n-1)^{(n-1)}e^{(1-n)}$$

A modification results in a cascade where nV = total cascade volume is constant (nτ = total cascade detention time also is constant) allows visualization of increasing dispersion in a single non-ideal reactor. So as n increases, V (single CSTR volume) decreases to keep nV constant. As n → ∞, V → 0 and cascade behavior approaches ideal plug flow.

$$C_n = \left(\frac{n}{(n-1)!}\right)\left(\frac{nt}{\tau}\right)^{(n-1)} e^{\left(\frac{-nt}{\tau}\right)}$$



CSTR Cascade, n-increasing, nV increasing
1
0.8
0.6
0.4
0.2
0
C_Tn/C_TO
0
2
4
6
8
10
t/τ
n = 1
n = 2
n = 3
n = 4
n = 5
n = 6

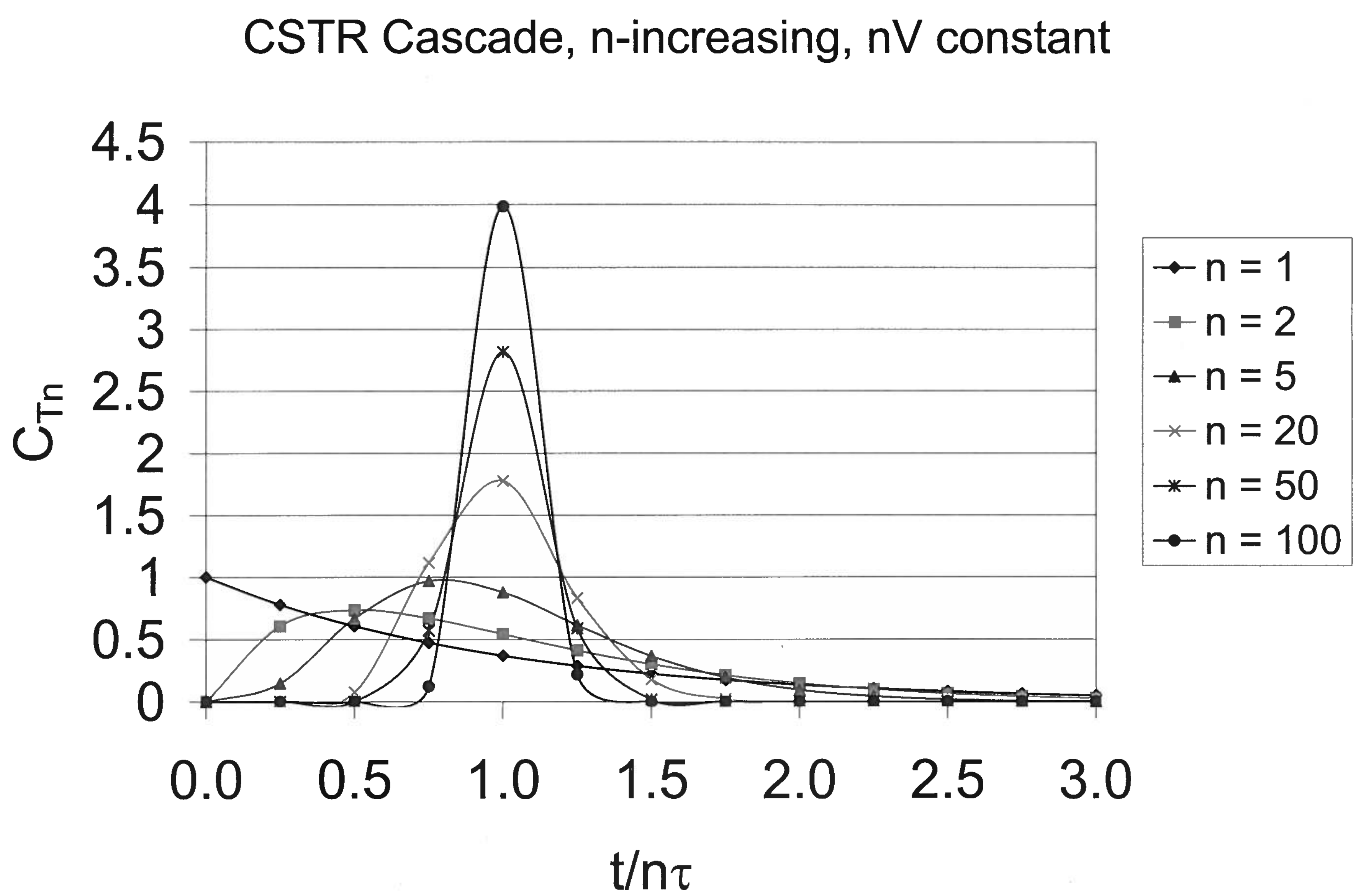
5A

CSTR Cascade
tank volume constant, cascade volume increasing as n increases
(I.e., like adding more CSTR tanks to end of cascade)

$C_{Tn}/C_{TO} = [1/(n-1)!]*(t/\tau)^{(n-1)}*\exp(-t/\tau)$

t/τ	C_{Tn}/C_{TO} n = 1	C_{Tn}/C_{TO} n = 2	C_{Tn}/C_{TO} n = 3	C_{Tn}/C_{TO} n = 4	C_{Tn}/C_{TO} n = 5	C_{Tn}/C_{TO} n = 6
0.00	1	0	0	0	0	0
0.25	0.778801	0.1947	0.0243	0.0020	0.0001	6.E-06
0.50	0.606531	0.3033	0.0758	0.0126	0.0016	0.0002
0.75	0.472367	0.3543	0.1329	0.0332	0.0062	0.0009
1.00	0.367879	0.3679	0.1839	0.0613	0.0153	0.0031
1.25	0.286505	0.3581	0.2238	0.0933	0.0291	0.0073
1.50	0.22313	0.3347	0.2510	0.1255	0.0471	0.0141
1.75	0.173774	0.3041	0.2661	0.1552	0.0679	0.0238
2.00	0.135335	0.2707	0.2707	0.1804	0.0902	0.0361
2.25	0.105399	0.2371	0.2668	0.2001	0.1126	0.0506
2.50	0.082085	0.2052	0.2565	0.2138	0.1336	0.0668
2.75	0.063928	0.1758	0.2417	0.2216	0.1523	0.0838
3.00	0.049787	0.1494	0.2240	0.2240	0.1680	0.1008
3.25	0.038774	0.1260	0.2048	0.2218	0.1802	0.1172
3.50	0.030197	0.1057	0.1850	0.2158	0.1888	0.1322
3.75	0.023518	0.0882	0.1654	0.2067	0.1938	0.1453
4.00	0.018316	0.0733	0.1465	0.1954	0.1954	0.1563
4.25	0.014264	0.0606	0.1288	0.1825	0.1939	0.1648
4.50	0.011109	0.0500	0.1125	0.1687	0.1898	0.1708
4.75	0.008652	0.0411	0.0976	0.1545	0.1835	0.1743
5.00	0.006738	0.0337	0.0842	0.1404	0.1755	0.1755
5.25	0.005248	0.0275	0.0723	0.1266	0.1661	0.1744
5.50	0.004087	0.0225	0.0618	0.1133	0.1558	0.1714
5.75	0.003183	0.0183	0.0526	0.1008	0.1450	0.1667
6.00	0.002479	0.0149	0.0446	0.0892	0.1339	0.1606
6.25	0.00193	0.0121	0.0377	0.0786	0.1227	0.1534
6.50	0.001503	0.0098	0.0318	0.0688	0.1118	0.1454
6.75	0.001171	0.0079	0.0267	0.0600	0.1013	0.1367
7.00	0.000912	0.0064	0.0223	0.0521	0.0912	0.1277
7.25	0.00071	0.0051	0.0187	0.0451	0.0818	0.1185
7.50	0.000553	0.0041	0.0156	0.0389	0.0729	0.1094
7.75	0.000431	0.0033	0.0129	0.0334	0.0647	0.1004
8.00	0.000335	0.0027	0.0107	0.0286	0.0573	0.0916
8.25	0.000261	0.0022	0.0089	0.0245	0.0504	0.0832
8.50	0.000203	0.0017	0.0074	0.0208	0.0443	0.0752
8.75	0.000158	0.0014	0.0061	0.0177	0.0387	0.0677
9.00	0.000123	0.0011	0.0050	0.0150	0.0337	0.0607
9.25	9.61E-05	0.0009	0.0041	0.0127	0.0293	0.0542
9.50	7.49E-05	0.0007	0.0034	0.0107	0.0254	0.0483
9.75	5.83E-05	0.0006	0.0028	0.0090	0.0220	0.0428
10.00	4.54E-05	0.0005	0.0023	0.0076	0.0189	0.0378

peak C_T^* @ $\frac{t}{\tau} = n-1$


CSTR Cascade, n-increasing, nV constant
C_Tn
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
t/nτ
n = 1
n = 2
n = 5
n = 20
n = 50
n = 100

5C

CSTR Cascade
system volume (nV) constant, tank volume decreasing as tank number increases
note that CTO also increases since "pulse" is first tank filled with dye (pulse mass is constant)
$C_{Tn} = (n/(n-1)!)*((n*t/\tau)^{(n-1)})*\exp(-nt/\tau)$

$t/n\tau$	C_{Tn} n = 1	C_{Tn} n = 2	C_{Tn} n = 5	C_{Tn} n = 20	C_{Tn} n = 50	C_{Tn} n = 100
0.00	1	0	0	0	0	0
0.25	0.7788	0.6065	0.1457	0.0000	0.0000	0.0000
0.50	0.6065	0.7358	0.6680	0.0746	0.0004	0.0000
0.75	0.4724	0.6694	0.9689	1.1149	0.5706	0.1227
1.00	0.3679	0.5413	0.8773	1.7767	2.8163	3.9861
1.25	0.2865	0.4104	0.6137	0.8307	0.5883	0.2174
1.50	0.2231	0.2987	0.3646	0.1788	0.0166	0.0002
1.75	0.1738	0.2114	0.1935	0.0225	0.0001	0.0000
2.00	0.1353	0.1465	0.0946	0.0019	3.E-07	9.E-14
2.25	0.1054	0.1000	0.0434	0.0001	4.E-10	2.E-19
2.50	0.0821	0.0674	0.0190	6.E-06	2.E-13	7.E-26
2.75	0.0639	0.0450	0.0080	2.E-07	9.E-17	1.E-32
3.00	0.0498	0.0297	0.0032	9.E-09	3.E-20	9.E-40
3.25	0.0388	0.0195	0.0013	3.E-10	5.E-24	4.E-47
3.50	0.0302	0.0128	0.0005	7.E-12	7.E-28	8.E-55
3.75	0.0235	0.0083	0.0002	2.E-13	7.E-32	1.E-62
4.00	0.0183	0.0054	0.0001	4.E-15	6.E-36	8.E-71
4.25	0.0143	0.0035	3.E-05	9.E-17	5.E-40	5.E-79
4.50	0.0111	0.0022	9.E-06	2.E-18	3.E-44	2.E-87
4.75	0.0087	0.0014	3.E-06	3.E-20	2.E-48	5.E-96
5.00	0.0067	0.0009	1.E-06	6.E-22	7.E-53	1.E-104
5.25	0.0052	0.0006	4.E-07	1.E-23	3.E-57	2.E-113
5.50	0.0041	0.0004	1.E-07	2.E-25	1.E-61	3.E-122
5.75	0.0032	0.0002	5.E-08	3.E-27	3.E-66	3.E-131
6.00	0.0025	0.0001	2.E-08	4.E-29	1.E-70	3.E-140
6.25	0.0019	0.0001	5.E-09	6.E-31	3.E-75	2.E-149
6.50	0.0015	0.0001	2.E-09	8.E-33	7.E-80	2.E-158
6.75	0.0012	4.E-05	6.E-10	1.E-34	2.E-84	1.E-167
7.00	0.0009	2.E-05	2.E-10	2.E-36	4.E-89	5.E-177
7.25	0.0007	1.E-05	6.E-11	2.E-38	8.E-94	2.E-186
7.50	0.0006	9.E-06	2.E-11	3.E-40	2.E-98	0.E+00
7.75	0.0004	6.E-06	7.E-12	3.E-42	3.E-103	0.E+00
8.00	0.0003	4.E-06	2.E-12	4.E-44	5.E-108	0.E+00
8.25	0.0003	2.E-06	7.E-13	5.E-46	8.E-113	0.E+00
8.50	0.0002	1.E-06	2.E-13	6.E-48	1.E-117	0.E+00
8.75	0.0002	9.E-07	8.E-14	7.E-50	2.E-122	0.E+00
9.00	0.0001	5.E-07	2.E-14	8.E-52	3.E-127	0.E+00
9.25	0.0001	3.E-07	8.E-15	9.E-54	4.E-132	0.E+00
9.50	0.0001	2.E-07	2.E-15	1.E-55	6.E-137	0.E+00
9.75	0.0001	1.E-07	8.E-16	1.E-57	8.E-142	0.E+00
10.00	5.E-05	8.E-08	3.E-16	1.E-59	1.E-146	0.E+00

peak closer to $t/n\tau = 1$ (like PFR)

CASCADE SIMULATION OF NON-IDEAL REACTOR WITH REACTION

For reaction A → B, let $r_A = -kC_A$ (1^{st} order reaction).

Steady state mass balance with influent = $C_{A,O}$

Tank 1:

$$QC_{A,O} - VkC_{A,1} = QC_{A,1}$$

$$C_{A,O} - k\tau C_{A,1} = C_{A,1}$$

$$\frac{C_{A,1}}{C_{A,O}} = \frac{1}{(1 + k\tau)}$$

Tank 2:

$$QC_{A,1} - VkC_{A,2} = QC_{A,2}$$

$$C_{A,1} - k\tau C_{A,2} = C_{A,2}$$

$$\frac{C_{A,O}}{(1 + k\tau)} = C_{A,2}(1 + k\tau)$$

$$\frac{C_{A,2}}{C_{A,O}} = \frac{1}{(1 + k\tau)^2}$$

Tank 3:

$$QC_{A,2} - VkC_{A,3} = QC_{A,3}$$

$$C_{A,2} - k\tau C_{A,3} = C_{A,3}$$

$$\frac{C_{A,O}}{(1 + k\tau)^2} = C_{A,3}(1 + k\tau)$$

$$\frac{C_{A,3}}{C_{A,O}} = \frac{1}{(1 + k\tau)^3}$$

Tank n:

$$\frac{C_{A,n}}{C_{A,O}} = \frac{1}{(1+k\tau)^n}$$

Rearranging,

$$\left(\frac{C_{A,n}}{C_{A,O}}\right)^{\frac{1}{n}} = \frac{1}{(1+k\tau)}$$

Solving for τ (single CSTR), given a level of fraction of A remaining in effluent, number of tanks, n, and rate constant k:

$$\tau = \frac{1}{k}\left[\left(\frac{C_{A,n}}{C_{A,O}}\right)^{\frac{-1}{n}} - 1\right]$$

And volume of entire reactor simulated by cascade required for conversion, nV, given the fraction of A remaining, number of CSTRs in series, and rate constant, k, where nV = nτQ:

$$nV = \frac{nQ}{k}\left[\left(\frac{C_{A,n}}{C_{A,O}}\right)^{\frac{-1}{n}} - 1\right]$$

Note that for a non-ideal reactor with a 1st-order reaction, simulated by the CSTR cascade model, the fraction of reactant, A, remaining is a function of n, as is the total reactor volume required for a given level of performance, nV.

Cascade simulation with zero-order kinetics: $r_A = -k$

Tank 1:

$$QC_{A,O} - Vk = QC_{A,1}$$

$$C_{A,1} = C_{A,O} - k\tau$$

Tank 2:

$$C_{A,2} = C_{A,1} - k\tau = C_{A,O} - k\tau - k\tau$$
$$C_{A,2} = C_{A,O} - 2k\tau$$

Tank n:

$$C_{A,n} = C_{A,O} - nk\tau$$

Note that the fraction of A remaining in the effluent, $\frac{C_{A,n}}{C_{A,O}}$, is a function of the influent concentration, unlike the first-order reaction behavior.

$$\frac{C_{A,n}}{C_{A,O}} = 1 - \frac{nk\tau}{C_{A,O}}$$

Solving for system volume, nV, required to achieve conversion ($C_{A,O} - C_{A,n}$), given k:

$$nV = \left(\frac{Q}{k}\right)\left(C_{A,O} - C_{A,n}\right)$$

For a non-ideal reactor with a zero-order reaction, note that the total reactor volume required for a given amount of conversion of reactant A IS NOT a function of n.

Cascade performance simulation for non-ideal reactors with more complex reaction rate models can be solved numerically as is done in wastewater process analysis software packages such as BioWin.

CASCADE SIMULATION OF NON-IDEAL REACTOR

First-order reaction

Showing effect of number of CSTRs in series and removal of reactant A

CONDITION: (Q/k) = 1

$V = ((C_{A,n}/C_{A,O})^{(-1/n)}-1)$

$nV = n*((C_{A,n}/C_{A,O})^{(-1/n)}-1)$

% A consumed	**fraction A remaining ($C_{A,n}/C_{A,O}$)**	**V, given n = 1, 2, 4, or 8**			
		1	2	4	8
99	0.01	99	9.0	2.2	0.78
90	0.10	9	2.2	0.8	0.33
50	0.50	1	0.4	0.2	0.09

% A consumed	**fraction A remaining ($C_{A,n}/C_{A,O}$)**	**nV, given n = 1, 2, 4, or 8**			
		1	2	4	8
99	0.01	99	18.0	8.6	6.23
90	0.10	9	4.3	3.1	2.67
50	0.50	1	0.8	0.8	0.72