

# Residence Time Distribution: Literature Survey, Functions, Mathematical Modeling, and Case Study – Diagnosis for a Photochemical Reactor

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**Table S1.** Dankwerts' works, followers, and contributors to RTD methodology progress

Name	Period/year	Representative study	Other works
Dankwerts P. V.	1950 - 1960	Continuous flow systems. Distribution of residence times [1], reprinted in 1995 [2]	[3-6]
Zwietering Th. N.	1959	The degree of mixing in continuous flow systems [7]	[8]
Bischoff K. B. and McCracken, E. A.	1966	Tracer tests in flow systems [9]	[10]
Cholette A. and Cloutier L.	1960 - 1970	Mixing efficiency determinations for continuous flow systems [11]	[12-14]
Levenspiel O.	1960 –1970 2011	Tracer curves and the residence time distribution [15]	[16-21]
Shinnar R.	1960 –1970 1993	Representation and Evaluation of Residence Time Distributions [22]	[23-25]
Buffham B. A.	1970 - 1990	The washout curve, residence-time distribution, and F curve in tracer kinetics [26]	[27-36]
Gibilaro L. G.	1970 - 1980	On the residence time distribution for systems with open boundaries [37]	[32,33,38,39]
Nauman E. B.	1970 – 1990 2008	Residence Time Theory [40]	[36,41-48]
Martin A. D.	2000	Interpretation of residence time distribution data [49]	[50]
Leclerc J. P., et al.	2000	Theoretical interpretation of residence-time distribution measurements in industrial processes [51]	[51-53]

**Table S2.** Prominent chemical engineering student's textbooks covering RDT methodology\*

Authors/Editors	Title	Vol./Ed.	Year	Ref. no
Levenspiel, O.	Chemical reaction engineering	3 <sup>rd</sup> Ed.	1998	[54]
Schmidt, L. D.	The engineering of chemical reactions	2 <sup>nd</sup> Ed.	2005	[55]
Nauman, E. B.	Chemical reactor design, optimization, and scaleup	2 <sup>nd</sup> Ed.	2008	[56]
Fogler, S. H.	Essentials of Chemical Reaction Engineering	1 <sup>st</sup> Ed.	2010	[57]
	Elements of chemical reaction engineering	4 <sup>th</sup> Ed.	2016	[58]
Green, D. W. and Southard, M. Z	Perry's Chemical Engineers' Handbook	8 <sup>th</sup> Ed.	2019	[59]
Ravi, R.; Vinu, R. G.; Sathyanarayana, N.	Coulson and Richardson's Chemical Engineering	Vol. 3/4 <sup>th</sup> Ed.	2017	[60]

\*Only the last editions are chronologically reported.

**Table S3.** Residence time distribution reviews in various industrial fields

Authors	Title	Year	Area of application	Ref. no.
Swaine, D. E. and Daugulis, A. J.	Review of Liquid Mixing in Packed Bed Biological Reactors	1988	Bioreactors	[61]
Ramaswamy, H. S et al.	Residence time distribution (RTD) in aseptic processing of particulate foods: a review	1995		[62]
Torres, A. P. and Oliveira, F. A. R.	Residence time distribution studies in continuous thermal processing of liquid foods: a review	1998	Food processing	[63]
Ganjyal, G. and Hanna, M.	A Review on Residence Time Distribution (RTD) in Food Extruders and Study on the Potential of Neural Networks in RTD Modeling	2002		[64]
Gao, Y. et al.	A review of the Residence Time Distribution (RTD) applications in solid unit operations	2012	Solid particles processing	[65]
Leray, E. et al.	Residence time distributions for hydrologic systems: Mechanistic foundations and steady-state analytical solutions	2016	Hydrology	[66]
Sheoran, M. et al.	Residence time distribution studies using radiotracers in chemical industry – A review	2018	RTD diagnosis using radiotracers in various industries	[67]
Bérard, A. et al.	Experimental methods in chemical engineering: Residence time distribution – RTD	2020	Chemical engineering	[68]
Reis M.H. et al.	The Influence of Residence Time Distribution on Continuous-Flow Polymerization	2019	Polymers	[69]
Bhalode, P. et al.	Using residence time distribution in pharmaceutical solid dose manufacturing – A critical review	2021	Pharmaceutics	[70]

Stephenson, R. and Sheridan, C.	Review of experimental procedures and modelling techniques for flow behaviour and their relation to residence time in constructed wetlands	2021	Wetland modelling	[71]
Rodrigues, A. E.	Experimental methods in chemical engineering: Residence time distribution—RTD	2021	Chemical engineering	[72]
Wang Z. et al.	Residence Time Distribution (RTD) Applications in Continuous Casting Tundish: A Review and New Perspectives	2022	Metallurgy	[73]
Ding, C. et al.	Challenge of Residence Time Distribution Curve in Tundish for Continuous Casting of Steel	2022		[74]
Sarkar M. et al.	Application of tracer technology in wastewater treatment processes: a review	2023	Wastewater treatment	[75]
Cherkasov, N. et al.	Continuous stirred tank reactors in fine chemical synthesis for efficient mixing, solids-handling, and rapid scale-up	2023	Chemical engineering	[76]

**Table S4.** Typical dimensionless numbers used in RTD analysis

Formula	Representative relations	Observations	Ref. no.
$Pe = \frac{v \cdot l}{D}$	$E(\theta) = \frac{\sqrt{Pe}}{2 \cdot \sqrt{\pi \cdot \theta}} \cdot \exp\left(-\frac{Pe \cdot (1 - \theta^2)}{4 \cdot \theta}\right)$ (standard dispersion model)	$Pe = Bo \cdot \frac{L}{l}$	[72,77]
$Bo = \frac{v \cdot L}{D_{ax}}$	$\sigma_{\theta}^2 = \frac{\sigma^2}{\tau^2} = \frac{2}{Bo} + \frac{8}{Bo^2}$ (open-open boundaries)	$Bo \rightarrow \infty$ plug flow	[78,79]
	$\sigma_{\theta}^2 = \frac{\sigma^2}{\tau^2} = \frac{2}{Bo} - \frac{2}{Bo^2} \cdot (1 - e^{Bo})$ (closed – closed boundaries)	$Bo \rightarrow 0$ perfectly mixed flow	[80]
$Da_1 = k \cdot t$ first order reaction	$\eta = 1 - \frac{4 \cdot q \cdot \exp\left(\frac{Pe}{2}\right)}{(1+q)^2 \cdot \exp\left(\frac{Pe \cdot q}{2}\right) - (1-q)^2 \cdot \exp\left(-\frac{Pe \cdot q}{2}\right)}$	If $Da < 0.1$ then $\eta < 0.1$	[58]
$Da_2 = k \cdot C_A^0 \cdot t$ second order reaction	$q = \sqrt{1 + \frac{4 \cdot Da}{Pe}}$ (closed – closed boundaries, first-order reaction)	If $Da > 10$ then $\eta > 0.9$	

where  $v$  represents flow velocity;  $L$  represents the systems length;  $l$  represents the characteristic length;  $D_{ax}$  = axial dispersion coefficient;  $D$  = mass diffusion coefficient,  $\eta$  = conversion

**Table S5** Representative non-ideal flow models

Name	Description	Parameters	Representative equation	Ref. no.
Cholette-Cloutier	The model associates a perfectly mixed tank, a bypass, and a dead zone. $V_D = (1 - \beta) \cdot V$	$\alpha, \beta$	$E(t) = \alpha \cdot \delta(t) + (1 - \alpha) \cdot \frac{(1 - \alpha)}{\beta \cdot t_s} \cdot \exp\left(-\frac{(1 - \alpha) \cdot t}{\beta \cdot t_s}\right)$ where $\delta(t)$ is Dirac delta function	[13,72]

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$$V_R = \beta \cdot V$$

Tank-in-series	<p>The model associates an "n" number of perfectly mixed, equal-volume tanks.</p> $M_v^0 = M_v^i = M_v^n$ $t_s = t_s^1 + \dots + t_s^i + \dots + t_s^n$	$n$ (or $N$ )	$E(\theta) = \frac{n^n}{(n-1)!} \cdot \theta^{n-1} \cdot e^{-\theta \cdot n}$ $F(\theta) = 1 - e^{-\theta \cdot n} \cdot \left[ 1 + \sum_{i=1}^n \frac{(n \cdot \theta)^{i-1}}{i!} \right]$ $\delta_\theta^2 = \frac{1}{n}$	[17,32,81,82]
Axial dispersion	<p>The model considers a plug flow that admits mixing and axial dispersion in the flow direction. System boundaries can be open, closed, or a combination of the two.</p> $C = f(t, z)$	$D_{ax}$	<p>If <math>n \rightarrow 0</math>, the series behaves as a perfectly mixed tank</p> <p>If <math>n \rightarrow \infty</math> the series behave as a plug flow</p> $E(\theta) = \frac{1}{2 \cdot \theta} \cdot \sqrt{\frac{Bo}{\pi \cdot \theta}} \cdot \exp\left(-\frac{(1-\theta)^2 \cdot Bo}{4 \cdot \theta}\right)$ <p>open – open boundaries</p> $E(\theta) = e^{\frac{Pe}{2}} \cdot \sum_{i=1}^{\infty} \frac{(-1)^{i+1} \cdot 8 \cdot \alpha_i^2 \cdot e^{\left(\frac{4 \cdot \alpha_i^2 + Pe^2}{4 \cdot Pe}\right)}}{Pe^2 + 4 \cdot Pe + 4 \cdot \alpha_i^2},$ <p>Where <math>\alpha_i</math> are the positive roots of the equation: <math>tg \alpha = \frac{4 \cdot Pe \cdot \alpha}{4 \cdot \alpha^2 - Pe^2}</math></p> <p>Closed – closed boundaries</p>	[82-84]

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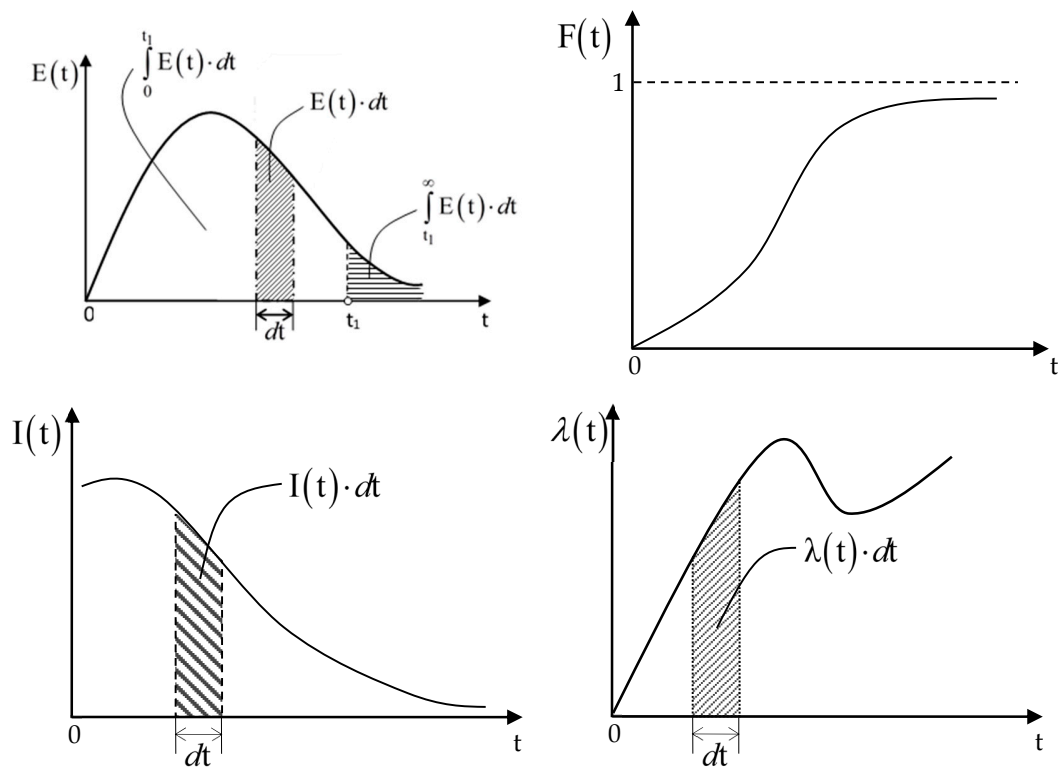
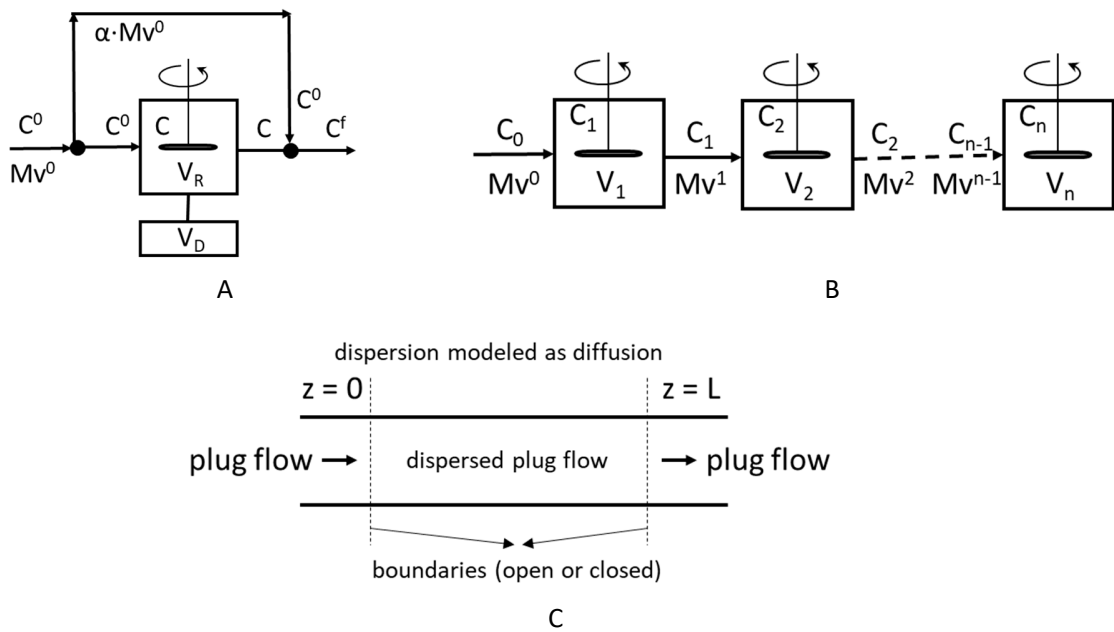
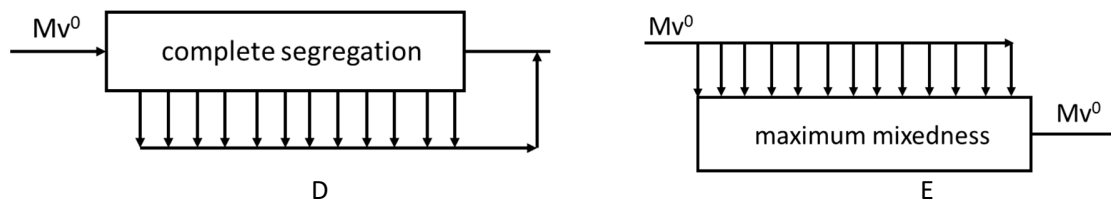


Figure S1. Typical RTD functions





**Figure S2.** Representative non-ideal flow and mixing models: **A:** Cholette-Cloutier model; **B:** Tank-in-series model; **C:** Axial dispersion model; **D:** Complete segregation model; **E:** Maximum mixedness model

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