Verification Examples

The Comparison between Published Experimental Data and Results of VisiMix Calculations

CONTENTS

These examples demonstrate the reliability of VisiMix simulation results by comparison with both published experimental data and the authors' original research.

EXAMPLE 1. Power Number - comparison with published and authors' experimental data

Agitator	Baffles	Power number		Source
		VisiMix calculations	Measurements	
Glaslock 90°	Standard	2.58 2.80	2.66 2.63	1 2
Glaslock 60°	Standard	2.03 2.23	1.84 1.88	1 2
Glaslock 45°	Standard	1.27 1.33	1.17 1.22	1 2
Glaslock 30°	Standard	0.69 0.72	0.62 0.68	1 2
Glaslock 90°	Thermometer Pocket	1.12	1.16	1
Glaslock 60°	Thermometer Pocket	0.95	0.94	1
Glaslock 45°	Thermometer Pocket	0.68	0.61	1
Glaslock 30°	Thermometer Pocket	0.42	46	1
Glaslock 90°	Beavertail- 3	2.17	2.16	2
Glaslock 90°	Beavertail- 2	1.74	1.82	2
Glaslock 30°	Beavertail- 2	0.56	0.49	2
Glaslock 30°	Beavertail- 1	0.47	0.415	2
Glaslock 30°	Beavertail- 3	0.60	0.64	2

Sources:

1 - Hattou S., Costes J. Recent Progres en Genie des Procedes, Vol.11, number 51 (1997), pp. 389-396.

2 - Authors' measurements, 1997.

EXAMPLE 2. Power and circulation flow rate for A200 and R100 impellers

(compared to experimental data of R. J. Weetman and J. Y. Oldshue, 6th European Conference on mixing, 1988).

Impeller	Power - measured, W	Power - VisiMix, W	Pumping capacity (Flow)- measured, m^3/s	Pumping capacity - VisiMix, m^3/s *	Total flow - measured, M^3/s **	Total flow - VisiMix, M^3/s**
A200	277	309	0.14	0.144	0.311	0.308
R100	334***	294	0.082	0.12	0.313	0.369

* For VisiMix data, it is calculated using the universally known relation:
Pumping capacity = Circulation flow rate /1.8.

** The Total flow is an integral value for meridional circulation and tangential flow velocities. The calculated value is based on VisiMix output parameters Circulation flow rate, Q, Average circulation velocity, V_{circ} and Average value of tangential velocity, V_{tg}:

Total flow = $Q * K$;

$$K = \frac{\sqrt{V_{circ}^2 + V_{tg}^2}}{V_{circ}}$$

***According to the values for the impeller diameter (406 mm), speed (101.8 RPM) and the experimental Power number of the R100 impeller presented in the article (5.13), this Mixing power value should be 285 W.

EXAMPLE 3. Circulation numbers for a pitch-blade impeller

(compared to experimental data of S. Gotz, R. Sperling et al., Chem. Eng. Technol., 20, 1997, 596-605).

D/T	Nq-experimental	Nq - VisiMix
0.4	1.3	1.37
0.36	1.55	1.57
0.3	1.75	2.0
0.25	2.0	2.75

The Circulation number, N_q (non-dimensional) is calculated as

$$N_q = \frac{q}{ND^3}$$

where q is circulation flow rate, m^3/s,
D is tip diameter of impeller, m,
N is RPM, 1/s

EXAMPLE 4. Mixing time

1. The comparison of Mixing time based on data reported by C.D. Riellt and R.E. Britter, Papers of the 5th European Conference on Mixing, Wurzburg, 1985, pp.365-375.

Conditions: Tank diameter - 290 mm,
Liquid height - 290 mm,
Rushton turbine, diameter 97mm
Number of revolutions - 6.7 1/s;

Measured values of mixing time: **4.2-4.6 s**.
VisiMix calculations: **5.55 s.**

2. The comparison of Mixing time for A315 agitator based on the article by K.L.Harrop et al. in the Proceedings of Mixing IX conference (Paris 1997), No.52, p.45, table 3 and the VisiMix results.

Conditions: Tank diameter -T =720 mm,
Liquid height - H = T
A315 agitator, diameter -D = 302 mm.

N, RPM	E, W/kg, Experimental	E, W/kg, VisiMix	Mixing time, measured, sec		Mixing time, VisiMix, sec	Characteristic time of micro-mixing, VisiMix, sec
			Conductivity	Decoloration		
100	0.038	0.035	19.3	26.6	24.8	6.6
150	0.128	0.117	12.3	16.7	16.6	3.6
200	0.293	0.278	9.3	11.5	12.4	2.34
250	0.544	0.542	7.3	10	9.92	1.68
300	0.921	0.937	7.3	8.0	8.27	1.28
350	1.421	1.490	6.7	7.5	7.09	1.01
400	2.123	2.13	5.3	5.8	6.2	0.83

3. The comparison of Mixing time values based on several correlations (see table below).

3.1. Correlation of A.Mersmann , W.-D. Einenkel and M. Kappel, Intern. Chem. Eng., v.16, p.590, 1976.

$$N\theta = 6.7\left(\frac{T}{D}\right)^{\frac{5}{7}} P_o^{-\frac{1}{3}}$$

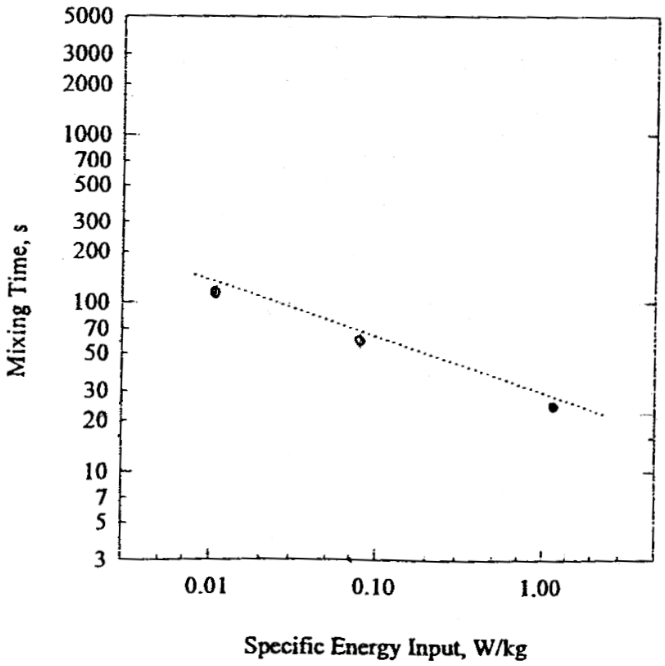
3.2. Correlation of S. Ruszkowski, Proc. 8th European Mixing Conf., I.Chem. E., 1994, p. 283, and R. K. Grenville, S. Ruszkowski and E. Garred, NAMF , Mixing XV, Namff, Canada, 1995:

$$N\theta = 5.3\left(\frac{T}{D}\right)^{2} P_o^{-\frac{1}{3}}$$

3.3. Data of FMP
3.4. VisiMix calculation (Total = Macromixing time + Micromixing time)

Impeller	Tank diameter, mm	Impeller diameter, mm	3.1 Mersmann 1976	3.2. Ruszkowski, Grenville 1994	3.3 FMP	3.4 VisiMix	
						Macro-mixing	Total
4 Pitch blade, 45°	1830	610	31.8	38.5	51.3-55.5	35.2	42.3
4 Pitch blade, 45°	1830	915	19.2	19.6	22-29	20.2	23.4
4 Flat blade	1830	610	29.2	32.6	42.4-66.6	46.3	54.6
4 Flat blade	1830	915	17.6	14.8	-	23.4	26.3

4. The comparison with the correlation of M. Cooke, J. C. Middleton and J. R. Bush, Proc. 2nd Int. Conf. Bioreactor Fluid Dynamics, BHRA/Elsevier, 37, 1988. The graph is reproduced from Fig. 5 in the article by A. H. John, W. Bujalski and A. W. Nienow, in the papers of Mixing IX conference (Paris 1997), No.52, p.169. Tank diameter is 750 mm, impeller diameter is 250 mm (according to the diagram in Figure 1), and the media level is 1500 mm.



Dotted line represents prediction of the M.Cooke's correlation for single 6DT.
Points correspond to VisiMix calculations.

EXAMPLE 5. Heat transfer coefficients (inside film coefficients)

Comparison of VisiMix calculations with correlations recommended by R.F.Dream, Chem. Engng, Jan. 1999, p.90-96.

Impeller	T/D	Impeller Re number	$Nu\ /(\Pr^{0.33}(\mu/\mu_w)^{0.14})$	
			Correlation	VisiMix 2000
Disk turbine	3	3000	158	121
		100000	1660	1650
6 Retreating blade	3	3000	145	116
		100000	1528	1600
Glass-lined impeller, 3 retreating blades	2	5000	111	100
		100000	1063	1121
Anchor	1.15	5000	165	193
		40000	670	650

The comparison of heat transfer coefficients calculated by VisiMix with experimental data is given in the Appendix.

EXAMPLE 6. Heat exchange coefficient: comparison with industrial results (ENI Chem, Italy)

This comparison was made in ENI Chem, Italy basing on their experimental data. The report concerns a CSTR batch. It is a process of dissolution of polybutadienic rubber (12% w/w) in liquid styrene consisting of the following main stages:

- introduction in the reactor of a fixed quantity of styrene
- introduction in the reactor of a fixed quantity of rubber and simultaneous heating (≅ 3h)
- dissolution of the rubber at costant temperature (≅ 7h)
- cooling of the batch (≅ 3 h)

During the 1991 commissioning some experimental transfer coefficient data were recorded:

DATE	HEATING	COOLING
13/02/91	154	150
	173	181
	150	167
14/02/91	199	-
	146	181
	198	-
AVERAGE 13/14	170	170

The average no fouling transfer coefficient calculated by VisiMix is (330 + 139)/2 = 230 W/m2°K (corresponding to 198 kCal/hm2°C). If we consider a jacket and process side fouling factors respectively of 0.0002 and 0.006 kCal/hm2°C, we obtain:

$$\mathbf{U\ overall} = \frac{\mathbf{1}}{\mathbf{1/198 + 0.0002 + 0.0006}} = \mathbf{165\ (kCal/hm2°C)}$$

The difference between the two average values is very low (<2%).

Conclusion:

The program is a valid working tool allowing a fast evaluation of some system's characteristics (thickness, Dp, speeds) very useful during the design. Heating and cooling times are very close to the actual with an approximation from 5% to 15%.

EXAMPLE 7. Comparison of local energy dissipation values calculated by VisiMix and measured by Genwen Zhou and Suzanne M. Kresta

The experimental data was borrowed from Impact of Tank Geometry on the Maximum Turbulence Energy Dissipation Rate for Impellers, AIChE Journal, September1996, Vol. 42, No.9, pp.2476 – 2490).

Notation:

N_f – number of baffles;
D - agitator tip diameter;
N – rotational speed;
Re – Reynolds number;
ε_{max} – maximum turbulence energy dissipation rate per unit mass at the outlet of impeller flow according to experimental data;
ε - average turbulence energy dissipation rate per unit mass calculated by VisiMix for the same area.
$Ve/Vv = (\varepsilon_{max}/\varepsilon)^{0.33}$ - ratio of pulsation velocities corresponding to ε_{max} and ε, respectively.

The results of the comparison between experimental data and results of the VisiMix calculations are presented in the tables below.

Pitch blade turbine

Experimental Data						VisiMix Results	
Run	N_f	D, mm	N, rpm	Re	ε_{max}, m^2/s^3	$\varepsilon, m^2/s^3$	$\mathbf{V_e/V_v}$
1	4	60	1133	66900	51.5	55	0.978
2	2	60	1133	66900	56.2	50	1.040
3	4	60	1133	66900	43.2	55	0.923
4	2	60	1133	66900	48.2	50	0.988
5	4	120	357	84300	12.0	6	1.260
6	2	120	357	84300	10.5	5	1.281
7	4	120	357	84300	10.1	12	0.944
8	2	120	357	84300	9.46	10	0.982
9	4	60	1133	66900	77.6	55	1.122

Pitch blade turbine

Experimental Data						VisiMix Results	
Run	N_f	D, mm	N, rpm	Re	ε_{max}, m^2/s^3	ε, m^2/s^3	**V_e/V_v**
10	2	60	1133	66900	69.1	50	1.079
N-1	4	80	357	35700	3.34	2.8	1.061
N-2	4	80	480	50400	7.71	7.0	1.033
N-3	4	80	580	60900	15.1	12.0	1.080
N-4	4	80	701	73600	23.8	22.0	1.027
N-5	4	80	800	84000	37.1	32.5	1.045

Lightnin A310

Experimental Data						VisiMix Results	
Run	N_f	D, mm	N, rpm	Re	ε_{max}, m^2/s^3	**ε,** m^2/s^3	**V_e/V_v**
1	4	84	1068	124000	30.2	20.2	1.14
2	2	84	1068	124000	28.1	19	1.14
3	4	84	1068	124000	25.9	20.2	1.09
4	2	84	1068	124000	20.9	19	1.03
5	4	132	503	144000	12.5	5.0	1.35
6	2	132	503	144000	11.6	4.8	1.34
7	4	132	503	144000	8.43	5.0	1.19
8	2	132	503	144000	8.16	4.8	1.20
9	4	84	1068	124000	26.1	20.2	1.09
10	2	84	1068	124000	18.6	19	1.0
N-1	4	114	430	91700	4.69	2.45	1.24
N-2	4	114	503	107000	7.36	3.8	1.24
N-3	4	114	570	122000	10.9	5.6	1.25
N-4	4	114	642	137000	15.2	8.0	1.24
N-5	4	114	720	153000	21.7	11.5	1.23

Rushton turbine

Experimental Data						VisiMix Results	
Run	N_f	D, mm	N, rpm	Re	ε_{max}, m^2/s^3	ε, m^2/s^3	V_e/V_v
1	4	60	714	42200	59.1	70	0.945
2	2	60	714	42200	81.7	70	1.053
3	4	60	714	42200	89.8	70	1.087
4	2	60	714	42200	84.3	70	1.064
5	4	120	225	53100	13.5	7	1.245
6	2	120	225	53100	9.42	6	1.162
7	4	120	225	53100	15.1	7	1.292
8	2	120	225	53100	13,8	6	1.320
9	4	60	714	42200	74.6	70	1.021
10	2	60	714	42200	74.6	70	1.021
N-1	4	80	225	23600	4.10	3.6	1.044
N-2	4	80	300	31500	9.73	8.2	1.059
N-3	4	80	442	38800	17.8	16.0	1.036
N-4	4	80	510	46400	31.4	28.0	1.039
N-5	4	80	800	53500	48.4	42.0	1.048

EXAMPLE 8. Sauter mean drop size in vessel with a disk turbine

Emulsion of chlorobenzene in water and NaCl solution. (Source: A.W. Pacek, C. C. Man and A.W. Nienow, C.E.Sc., v.53. No.11, p.2005, 1998).

Tank diameter –150 mm,
Impeller diameter – 75 mm,
Media: chlorobenzene in water,
Volume fraction of disperse phase – 0.05 – 10%.

The results of the comparison are shown in the table and graphs below.

Parameters of calculation error	Correlations of A. W. Pacek Number of constants based on experimental D_{32} values		VisiMix calculations Number of constants based on experimental D_{32} values	
	3	2	1 – Index of admixtures = -0.2	No constants. Index of admixtures = 0
A = D_{32}exp/ D_{32}calc, average value	1.00	1.15	0.999	1.007
Mean square root deviation	0.172	0.24	0.29	0.318

In the graphs, A represents measured values of Sauter mean drop size d_{32} (μm) based on the source, B represents calculated d_{32} (μm) values.

In Figure 1, calculations were performed according to experimental correlation proposed by Pacek et al. in the article cited above.

In Figure 2, calculations were performed with VisiMix for Index of admixtures equal to -0.2.

In Figure 3, calculations were performed with VisiMix (no experimental constants, Index of admixtures equal to 0).

Comparison of measured and calculated d_{32} values

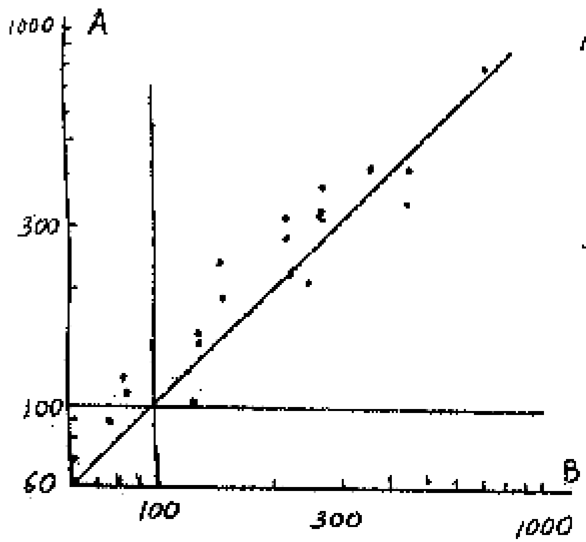


Figure 1.

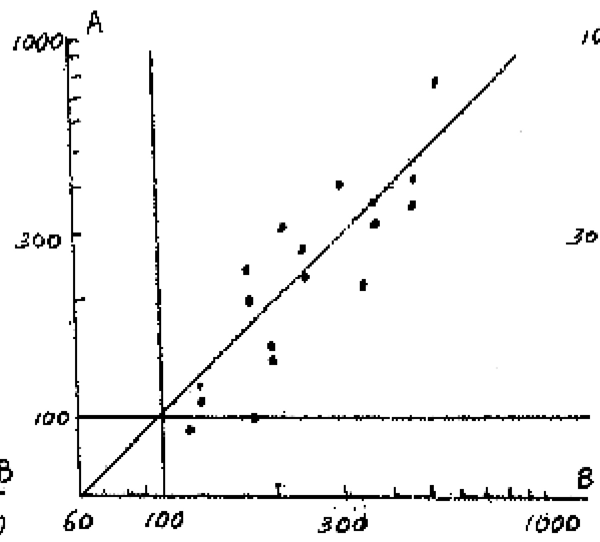


Figure 2.

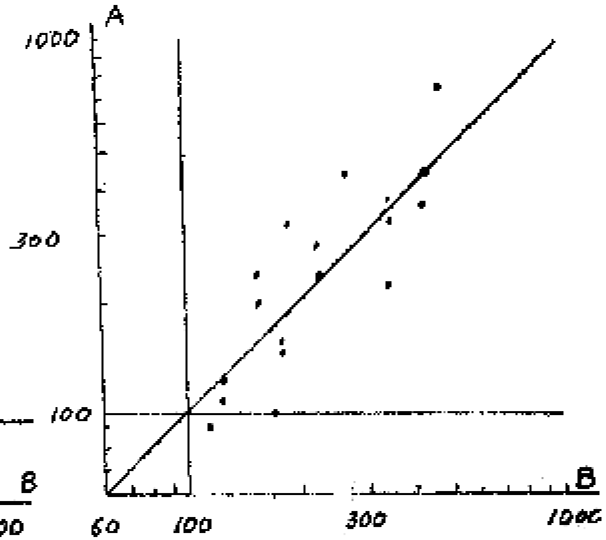


Figure 3.

EXAMPLE 9. Comparison of Sauter Drop Size values calculated by VisiMix and measured by Genwen Zhou and Suzanne M. Kresta

The experimental data was borrowed from Correlation of mean drop size and minimum drop size with the turbulence energy dissipation and the flow in an agitated tank**,** Genwen Zhou and Suzanne M. Kresta, *Department of Chemical Engineering, University of Alberta, Edmonton, Alberta, Canada, T6G 2G6.* Published in **Chemical Engineering Science,** Vol. 53, No 11, pp.2063-2079,1998.

The authors present data on the size of the drops, which form as a result of emulsification of silicon oil in water in vessels with several agitator types of different geometries and dimensions. The results of the comparison are given in the table below.

Mean Drop Size Values at Different Rotational Speeds

Impeller/geometry	N, 1/s	d_{32}, μm - measured	d_{32}, μm –VisiMix
A310 N_f = 4 D = 0.350T C/D=1 F(η) at 2r/D = 0.50	11.3 13.3 15.5 16.3 16.9 17.8 18.8 20.7 22.7	149.0 125.0 94.90 87.40 81.80 72.81 68.21 64.70 58.91	141 114 93.6 87.8 83.9 78.7 73.6 65.4 58.6
A310 N_f = 4 D = 0.550T C/D=1/2 F(η) at 2r/D = 0.55	7.67 8.22 8.78 9.43 10.5	117.5 104.7 93.10 81.20 60.20	138 126 117 107 93.9
PBT N_f = 4 D = T/4 C/D=1 F(η) at 2r/D = 0.30	16.4 17.2 18.4 20.0 22.4 24.1 26.4 30.0	117.8 109.6 100.0 89.51 73.42 62.32 55.91 50.72	104 98 89.4 80.3 69.6 63.5 56.8 48.7
RT N_f = 4 D = T/4 C/D=1 F(η) at 2r/D = 0.30	11.1 12.1 13.5 15.2 17.1 20.3	90.12 82.09 71.01 58.89 53.78 51.72	88.2 79.0 68.9 59.6 51.8 42.6
RT N_f = 4 D = T/4 C/D=1 F(η) at 2r/D = 0.30	8.62 9.92 11.4 13.4 15.5 17.6 19.2	111.0 96.61 86.02 73.49 61.39 51.02 44.53	124 102 85.3 69.5 58.2 50.1 45.4

Notation:

A310 Lightnin A310 impeller
PBT pitched blade turbine
RT Rushton turbine
N_f number of baffles
D impeller diameter
T tank diameter
C off bottom clearance
F(η) percentage of drops of a diameter smaller than Kolmogorov's scale of turbulence
r radial coordinate, m
d_{32} mean Sauter drop size
N rotational speed,

EXAMPLE 10: Just Suspension Speed (JSS)

In this example, VisiMix is used for determining "just suspension speed" (**JSS**). The example is based on experimental data presented by A. Mac, S.Yang, and N.G. Ozcan-Taskin in *The Effect of Scale on the Suspension and Distribution of Solids in Stirred Vessels* published in *Mixing IX, Multiphase Systems* , No.52, Vol. 11 - 1997, (Proceedings of the 9th European Conference on Mixing: MIXING 97), pp.97-104.

The basic requirement in all solid-liquid mixing processes is to avoid the formation of a stagnant zone of solid at the tank bottom. It means that design and operation parameters must ensure the "just suspension condition". The experiments described in the paper above were aimed at determining **JSS** and its dependence on scale and concentration of solids. All the experiments were performed with geometrically similar cylindrical fully baffled vessels with torispherical bottoms of the following diameters T: 0.30m (referred to as T30), 0.61m (T61), 1.83m (T183) and 2.67m (T267). Mixing was achieved by means of a downward pumping pitched blade turbine of diameter (D) equal to T/2 with 4 blades inclined at 45° installed at an off-bottom clearance of T/4.

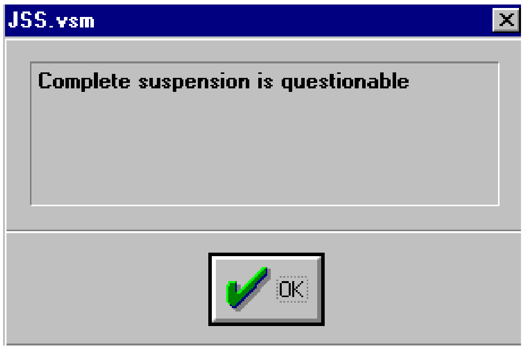
In-vessel media contained tap water and sand particles. The density of the latter was about 2630 kg/m^3, and the particle size was 150-210 microns. The slurry height (H) was equal to the vessel diameter (T).

The task is to calculate RPM value at which partial settling of the solid phase may occur.

Visimix Model

To analyze the problem, we must first enter design and process parameters, which is easy. The only difficulty lies in determining the corresponding experimental values of solid concentration, as they can be obtained only approximately from the graph with logarithmic scale given in the above mentioned paper.
The calculation procedure was as follows:

At first, wittingly high RPM values were entered at which no solid settling may happen. Then RPM numbers were gradually reduced until VisiMix issued the following message:

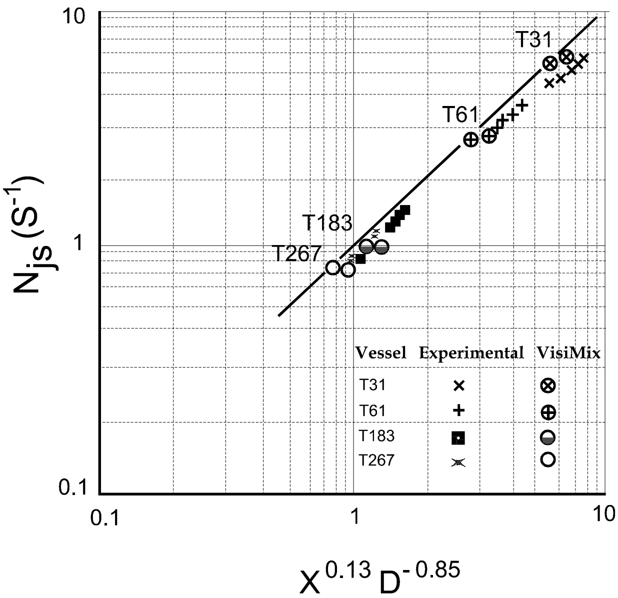


Visimix message informing the user that JSS value is reached.

The corresponding RPM value was taken as **JSS.**

Verification

Since exact values of solid concentration were unknown, the comparison of the Visimix simulation results and experimental data was performed by placing calculated data on the experimental graph.



The effect of solid concentration and scale on the JSS. Comparison between Visimix simulation and experimental data.

The graph shows excellent agreement between VisiMix and experimental data. According to our estimations, the deviation doesn't exceed 16%.

EXAMPLE 11. JSS in a laboratory tank with single and multi-stage 6 flat-blade impellers

(Source: P.M.Armenante and Tong Li, AIChE Symp. Ser., vol. 89, 1993, p.105).

Tank diameter – 292 mm, height – 330 mm;
Media: Water - Glass spheres , diameter – 110 mm.

Impeller diameter, Mm	Number of stages	Distance from bottom, mm	Distance between stages, mm	JSS, VisiMix, Rpm	JSS Measured, rpm*
65	1	32.5	-	710	700
76	1	38	-	555	510
102	1	51	-	350	300
65	3	51	102	725	800
76	3	51	102	575	575
102	3	51	102	375	325
65	3	32.5	102	719	720
76	3	38	102	566	530

* The measured values in this column are approximate, taken from graphs, Fig. 2a, b on p.106 in the source.

EXAMPLE 12. JSS in tanks with single-stage impellers

(Source – FMP report).

Tank diameter, mm	610	1830
Height of media, mm	610	1830
Type of agitator	A310	4 Pitch blade, 45^0
Impeller diameter, mm	305	930
Distance from bottom, mm	153	458
Liquid phase	Water	Water
Solid phase	Sand	Sand
Concentration, kg/cub. m	376	269
Density	2630	2630
Average part. size, mm	0.18	0.18
Impeller Power number		
Measured	0.29	1.7
VisiMix	0.29	1.56
JSS - measured	277	79
JSS – VisiMix	305	66

EXAMPLE 13. JSS in a laboratory tank with single pitch-blade disk turbine

(Source – D. Birch and N. Ahmed, in papers of the Mixing IX conference, Paris 1997, No.52, p.177).

Tank diameter – 600 mm, tank height – 600 mm.
Impeller: 6-blade Disk turbine, diameter 200 mm, pitch angle 45^0
Media: Water - Glass spheres, average diameter – 300 mm.

JSS Values:

Measured (in non-aerated conditions Fig. 5, agitator PDD): **4.5-5.5 RPM**
Calculated – **5.17 RPM.**

EXAMPLE 14. JSS in tanks with pitch blade impellers

(Source – C. Buurman, G. Resoort and A. Plaschkes, Chem.Eng.Sci., v.41, No.11, p.2865, 1986).

Tank diameter, mm	480	4260
Height of media, mm	480	4260
Type of agitator	4 Pitch blade, 45^0	4 Pitch blade, 45^0
Agitator diameter,mm	200	1720
Distance from bottom,mm	160	1420
Liquid phase	Water	Water
Solid phase	Sand	Sand
Concentration, kg/cub.m	100-400	100-400
Density	2630	2630
Average part. size, mm*	0.178	0.178
JSS – measured**	240-280	50-60
JSS – VisiMix	230-250	52-58

* The average particle size is based on results of a sieve analysis presented in the article.
** These values of measured Just Suspending Speed are estimated using the graphs in Figs 3 and 4 of the article.

EXAMPLE 15. Production of propylene glycol

This example shows VisiMix capabilities in simulating exothermic reaction. It is borrowed from the book of H. Scott Fogler, *Elements of Chemical Reaction Engineering*, 2nd ed. (Prentice-Hall, Inc. 1992), pp. 400 - 405, *Examples 8-4 and 8-5.*

Propylene glycol (**PG**) is produced by the hydrolysis of propylene oxide (**PO**). The reaction takes place at room temperature when catalyzed by sulfuric acid.

$$PO + H_2O \xrightarrow{H_2SO_4} PG$$

In accordance with the technological requirements, 2500 lb/h (43.03 lb mol/h) of **PO** is fed to the reactor. The feedstream consists of (**1**) an equivolumetric mixture of **PO** (46.62 ft^3/h) and **methanol** (46.62 ft^3/h), and (**2**) **water** containing 0.1 wt% **H_2SO_4**. The volumetric flow rate of **water** is 233.1 ft^3/h, which is 2.5 times **methanol - PO** flow rate. The corresponding molar feed rates of **methanol** and **water** are 71.87 and 802.8 lb mol/h, respectively. The inlet temperature of all feedstreams is 75°F. The reaction under consideration is first-order in propylene oxide concentration, and apparent zero-order in excess of water with the specific reaction rate

$\boldsymbol{k = A\, e}^{-E/RT} = 16.96 * 10^{\mathbf{12}} (\boldsymbol{e}^{\boldsymbol{-32400/RT}})\ \mathrm{h}^{-1}$

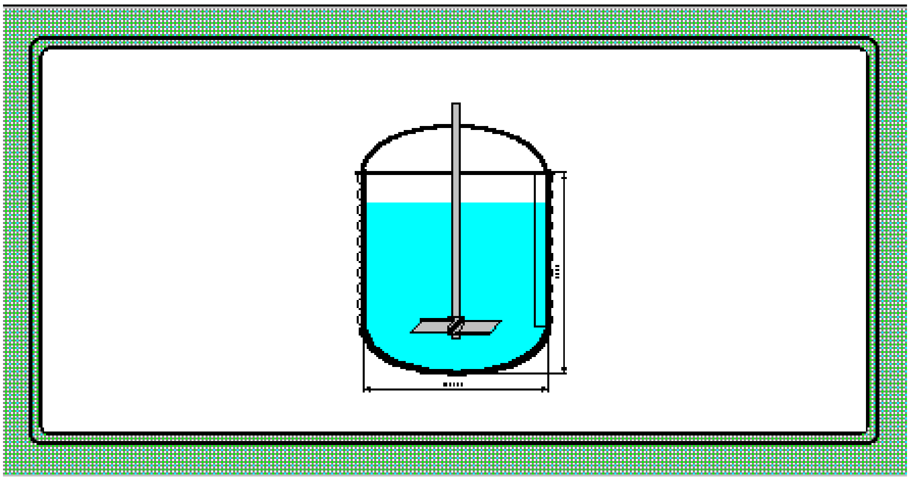
In this equation, the unit of ***E*** is Btu/lb mol.

The process has an important operating constraint. The temperature of the mixture must not exceed 125°F because of the low boiling point of **PO**.

The task is to find if this process can be realized in a glass-lined Continuos-Stirred Tank Reactor (**CSTR**) of 300-gal capacity. And if so, what will be the value of **PO/PG** conversion.

Visimix Model

The process was simulated as a steady-state of the transient occurring in the following conditions: CSTR is filled with water which is then expelled by two components: reactant **A** (**PO** with flow rate equal 46.62 ft^3/h of) and reactant **B**, which is actually a mixture of **methanol** (46.62 ft^3/h) and **water** containing 0.1 wt% $\mathbf{H_2SO_4}$ (233.1 ft^3/h). The properties of reactant **B** were assumed to be close to those of water. The diagram of the reactor is shown below:



CSTR diagram.

Verification

Visimix simulation was performed in order to obtain **PO-PG** conversion as a function of the in-tank media temperature. Calculations were done for several values of initial tank temperature, inlet feedstream temperature and inlet temperature of in-jacket heat transfer liquid. The results of the calculations, as compared with the data in H.S. Fogler's book quoted above, are given in the table below.

PO-PG conversion

Media Temperature, °R	Conversion (VisiMix)	Conversion (H.S. Fogler)
550	0.212	0.217
565	0.384	0.379
575	0.511	0.500
585	0.632	0.620
595	0.725	0.723
605	0.803	0.800

The comparison between VisiMix and reference data shows that they practically coincide with each other.

Note that the VisiMix approach, unlike the perfect reactor approach used by H.S. Fogler, is based on the imperfect reactor model. This enables us to take into account the effect of various design parameters (type and dimensions of agitator, baffle, jackets, as well as type and properties of in-jacket heat transfer fluid). The role of these parameters is especially important during transient calculations.

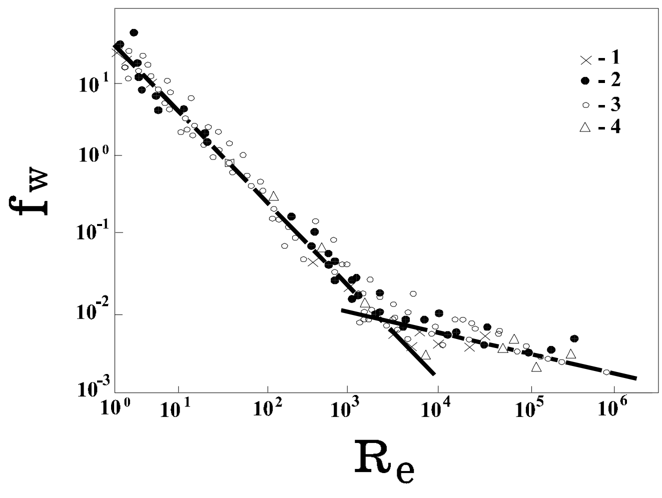
Examples from the Review of Mathematical Models Used in VisiMix,

VisiMix Ltd., Jerusalem, Israel, 1998.

1. Wall flow resistance factor

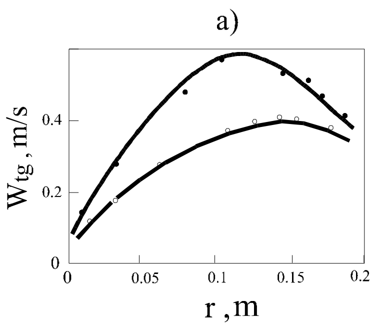
This example is given after Braginsky et al., Mixing of Liquids. Physical Foundations and Calculation Methods, Khimya Publishers, Leningrad (1984). It shows the measured and calculated values of wall flow resistance factor, f_w in tanks with different agitators. In the graph below, tank diameters were 0.3 to 1.0 m; agitators: 1, 2 - turbines; 3 - paddle; 4 - propeller. $R / R_{agt} \geq 2.0$. $Re = W_{av} R_T / \nu$.

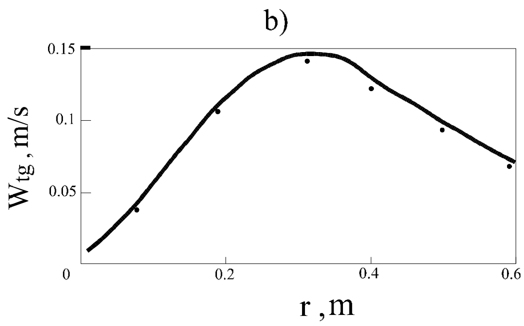
Solid lines correspond to the VisiMix calculations.



2. Tangential velocity profiles

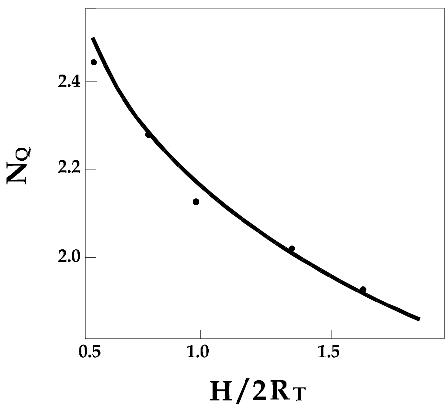
This example is taken from the same source as the one above. It shows experimental and calculated values of the tangential velocity, w_{tg} profiles for a) tank of diameter 0.4 m equipped with the frame agitator, and b) tank of diameter 1.2 m with the twin-blade agitator. The solid lines correspond to the VisiMix calculations.





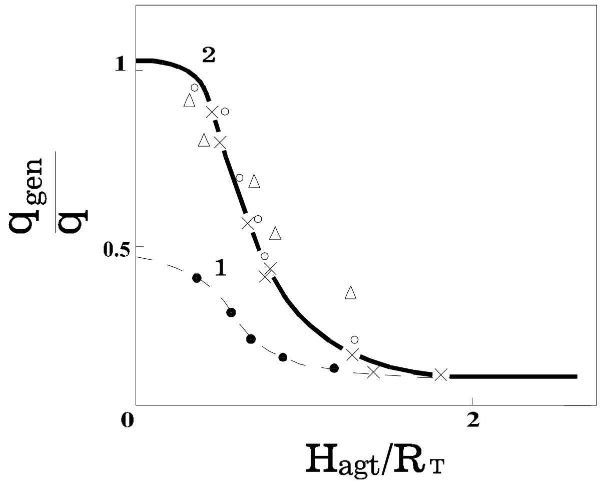
3. Circulation number

This example is taken from Yaroshenko, V., Braginsky, L. et al., *Theor. Found. of Chem. Eng.* (USSR), 22, 6 (1988, USA translation -1989). It shows experimental and calculated values for the circulation number, $N_0 = q/(n*D^3_{agt})$ as a function of the level of media in the tank. In the graph, tank diameter is 0.5 m; agitator is a disk turbine. The solid line corresponds to the VisiMix calculations.



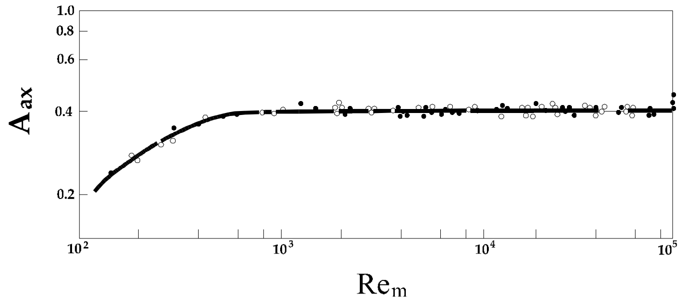
4. General circulation flow rate in a 2-stage mixing system

This example is based on experimental data reported by Fort I., J. Hajek and V. Machon, *Collect. Czech. Chem. Commun.*, 1989, v.34, pp 2345-2353, and by Braginsky et al., Mixing of Liquids. Physical Foundations and Calculation Methods, Khimya Publishers, Leningrad (1984). In multistage mixing systems, the axial circulation may be described as a superposition of two kinds of axial circulation cycles: local circulation cycles around each agitator, and a general circulation cycle which envelopes the total height of the tank. It has been found that the values of circulation flow rate for both kinds of cycles depend on the distance between agitators and are directly proportional to circulation flow rate, **q** for a single agitator of the same type and size. In the graph below, 1 is pitched-paddle agitator; 2 is disk turbine with vertical blades. The lines represent the VisiMix calculation.



5. The mixing length factor

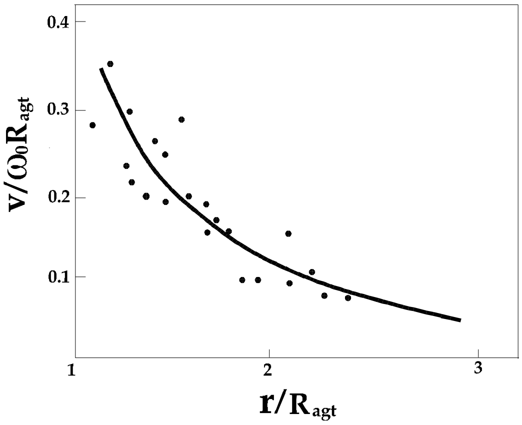
This example is based on experimental data from Braginsky et al., Mixing of Liquids. Physical Foundations and Calculation Methods, Khimya Publishers, Leningrad (1984). The points represent the results of measurements in different mixing conditions, in various equipment types and scales. We can see that all points lie on one line, and at Re numbers higher than 700, A_{ax} value remains constant. This brilliantly confirms the applicability of the Prandtl model of turbulence (mixing length hypothesis) to the description of flows in mixing tanks. Therefore, this model is used in VisiMix.



The mixing length factor, A_{ax} as a function of $Re_m = n * D^2_{agt} / \nu$.

6. Mean square root (MSR) velocity of turbulent pulsations

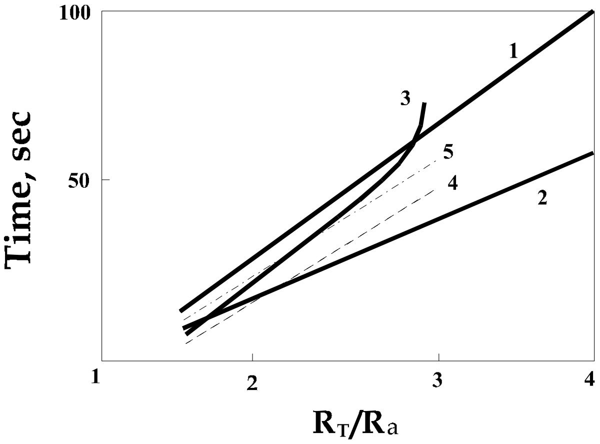
The experimental data for this example was taken from Costes J., J.F. Couderc, *Chem. Eng. Sci.*, 1987, v.42, N2, p.35-42. The solid line corresponds to the results of the simulation; the data points show published experimental results (disk turbine agitators).



V is RMS velocity, ω_0 is angular agitator velocity, r is current radius, and R_{agt} is agitator radius.

7. Macromixing time

The experimental data for this example was taken from the following publications:
Hiraoka S. and R. Ito, J. Chem. Eng. Japan, 1977, v.10, N1, p.75 – line 3 in the graph below
Shiue, S. J. and C.W. Wong, Canad. J. Chem. Eng., 1984, v.62, p.602 – line 4
Sano, Y. and H. Usui, J. Chem. Eng. Japan, 1985, 18, N1, p.47 - line 5. All data was obtained in tanks with disk turbine agitator (Rushton turbine).

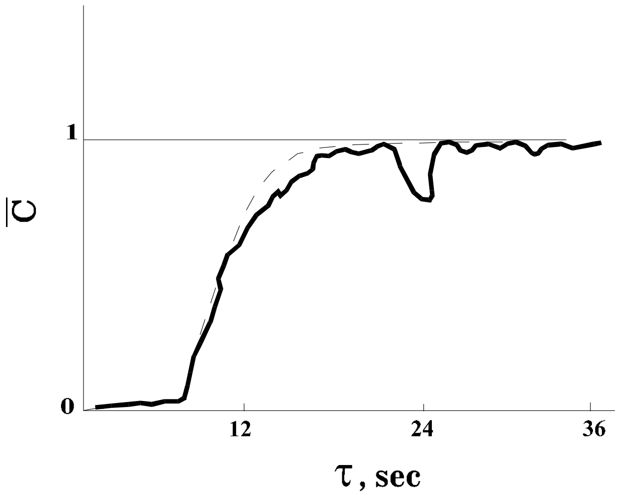


Solid lines 1 and 2 represent VisiMix calculations:
1 - micromixing time + macromixing time
2 – macromixing time only

R_T is the tank radius, R_a is the agitator radius.

8. Typical response curve for multistage agitator systems

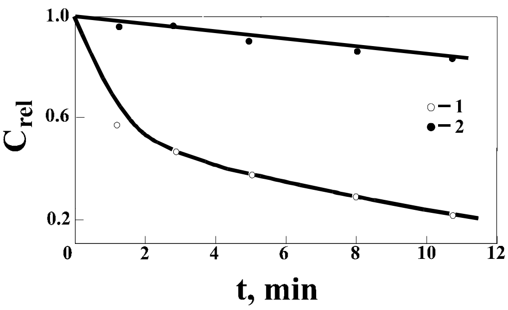
The experimental data for this example is derived from the authors' original research.



The graph shows the change in the tracer concentration in tank with 2-stage pitch paddle agitator (batch blending). Injection point - below the lower agitator, the sensor is located close to the surface of media. The solid line corresponds to the measured data, the dotted line corresponds to the results of simulation.

9. Local concentration of reactant in semibatch reactor

This example is based on experimental data from Braginsky et al., Mixing of Liquids. Physical Foundations and Calculation Methods, Khimya Publishers, Leningrad (1984).

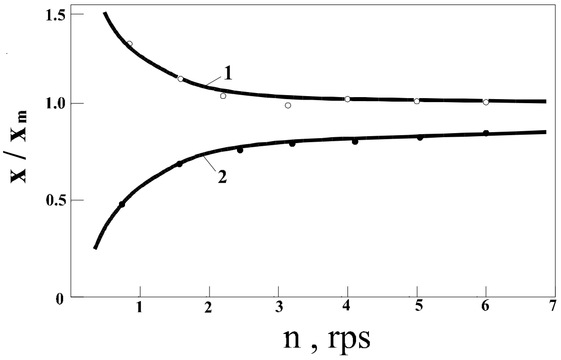


A fast reaction ($k_r \to \infty$); $C_{rel} = C_a/C_{a\,0}$. Tank diameter: 0.25 m; radius of agitator: (1) - r = 0.05 m; (2) - r = 0.11 m.

Solid lines represent calculations by VisiMix calculation models.

10. Local concentration of suspended particles

This example is based on experimental data from Braginsky et al., Mixing of Liquids. Physical Foundations and Calculation Methods, Khimya Publishers, Leningrad (1984), and Soo, S. The Hydrodynamics of Multiphase Systems (Transl.), Mir Publishers, Moscow, 1971. It shows experimental and calculated values for the concentration of silica gel in kerosene at *h/H*=0.1 (curve 1) and *h/H*=0.9 (curve 2) as a function of the rotational velocity of the agitator (tank diameter is 0.3; impeller, R_T/R_{agt} = 2.15; W_s = 0.00825 m/s). The solid lines correspond to the calculated values.



x is local concentration of the solid phase

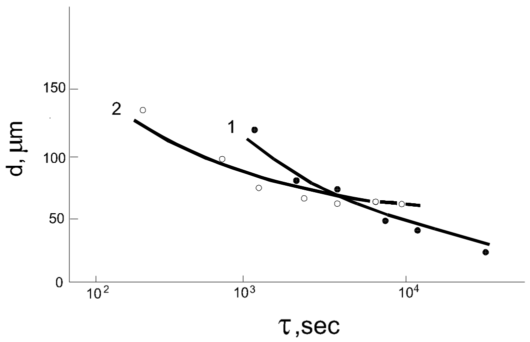
x_m is average concentration of the solid phase in the tank

n is rotational speed of the agitator

11. Mean drop size

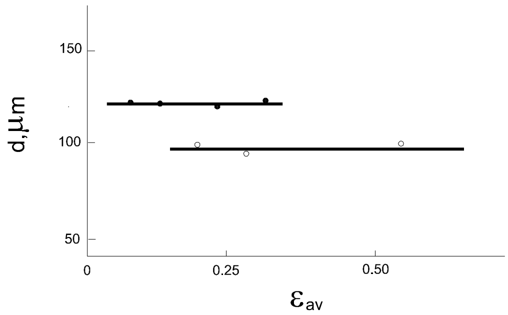
This example is based on experimental data from the paper by Braginsky, L. N. and Kokotov, Y. V., *Kinetics of Break-Up and Coalescence of Drops in Mixing Vessels* presented at CHISA, Prague, 1993, and published in the proceedings of LLFT-97, Antalya, Turkey, 1997, pp. 567-574.

Studies of breaking in non-coalescing systems (in the presence of corresponding emulsifiers) were carried out in vessels of three different volumes (up to 250 l) with 17 different agitators and 6 liquid couples. Relation of viscosities of phases varied by more than 600 times. In all graphs below, solid lines represent the VisiMix calculations.

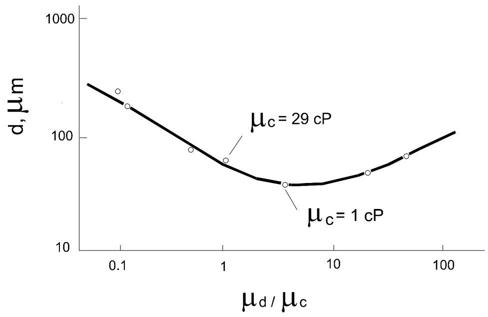


Kinetics of drop breaking in the absence of coalescence.

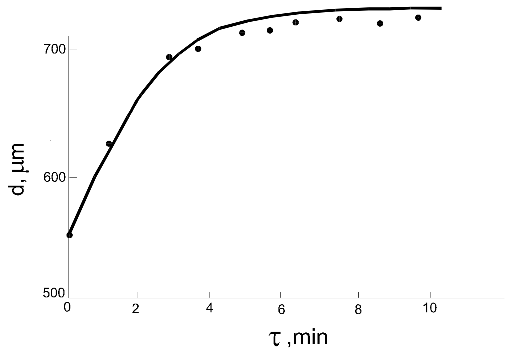
1 - 6-blade turbine, ε_m = 150 W/Kg, 2 -disk agitator, ε_m = 650 W/Kg.



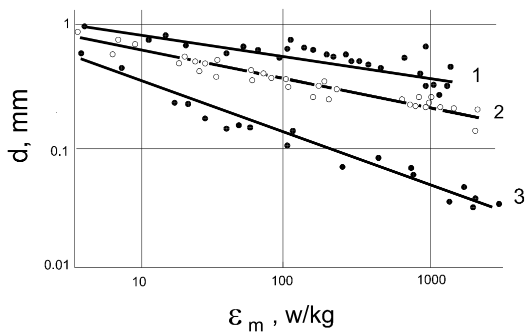
Break-up in the absence of coalescence. Mean drop size (“final” values) vs. specific power for different agitators. 1 - ε_m = 30 W/Kg, 2 - ε_m = 60 W/Kg.



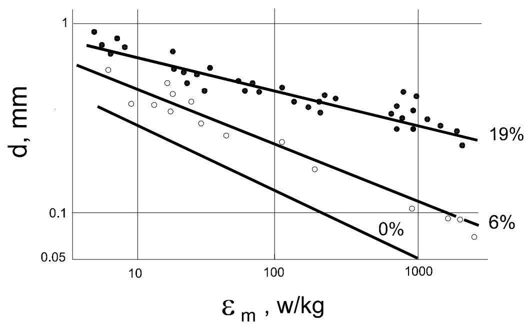
Break-up in the absence of coalescence. Mean drop size vs. relation of viscosities.



Kinetics of coalescence.
Agitator - 6-blade turbine, diameter 100 mm. φ=0.19. Rotational velocity changed from 240 to 160 RPM.



Break-up and coalescence. Mean drop diameter (“final” value) vs. ε_m .
1 - P = 20 Pa; 2 - P = 7 Pa; 3 - P $\rightarrow\infty$ (stabilized).



Break-up and coalescence. Mean drop diameter vs. ε_m . The effect of the concentration of the disperse phase.

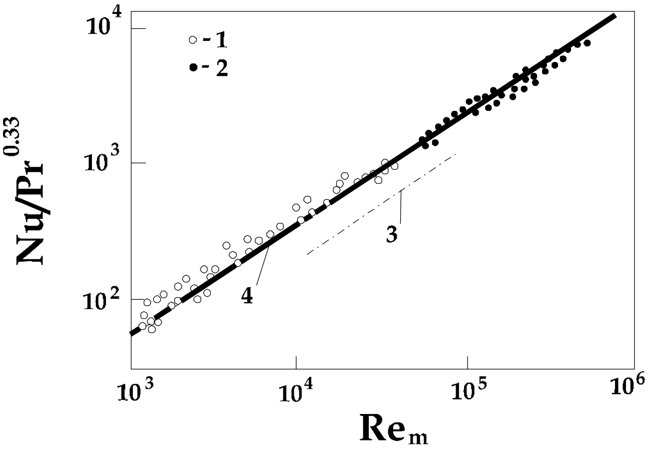
Notation:

d	mean drop diameter
ε_m	energy dissipation, maximum value
μ_d, μ_c	dynamic viscosities of disperse and continuos phases, respectively

11. Heat transfer coefficient

The experimental results for this example were taken from:

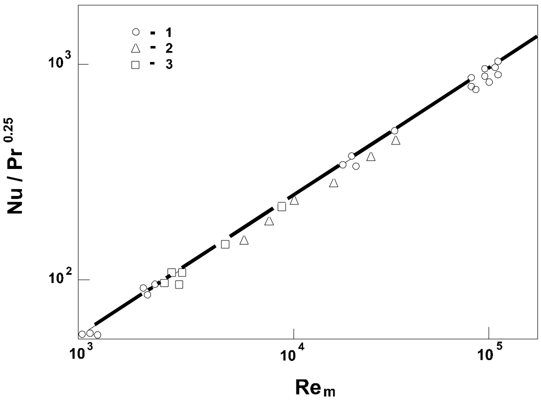
1. Barabash, V.M. and Braginsky, L. N., Eng. - Phys. Journal (USSR), 1981, v. 40, No.1, pp. 16-20.
2. Landau, L.D. and Lifshitz, E. M., Mechanics of Continuous Media, Gostechizdat Publishers, Moscow, 1953.
3. Levich, V.G., Physico-Chemical Hydrodynamics, Physmatgiz Publishers, Moscow, 1959.
4. Chapman, F., Dallenbac, H. and Holland, F., Trans. Inst. Chem. Eng., 1964, v. 42, pp. 398-403.
5. Strek, F., Chemia Stosowana , 1962, No.3, p.329.
6. Strek, F., Karcz, J. and Bujalki, W., Chem. Eng. Technol., 1990, v. 13, pp. 384-392.



Heat transfer in tanks with turbine disk agitators.

1 - [1]; 2 - [2] and 3 - [3]; 4 - results of VisiMix calculations.

Re_m	Impeller Reynolds number
Nu	Nusselt number
Pr	Prandtl number



Heat transfer in tanks with anchor type agitators.

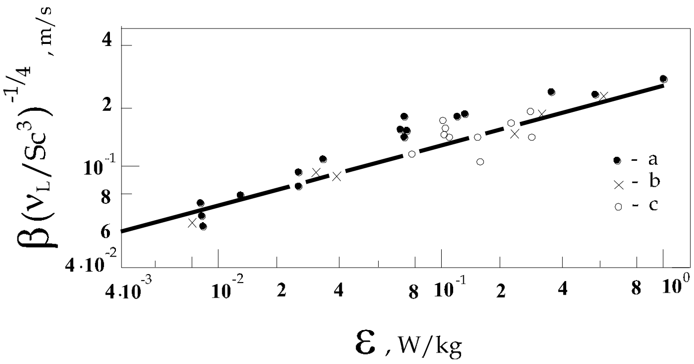
1 - [4]; 2 - [5]; 3 - [6]. The solid line represents results of VisiMix calculations.

Re_m Impeller Reynolds number
Nu Nusselt number
Pr Prandtl number

12. Mass transfer coefficient in suspension

Liquid-solid mass transfer coefficient as a function of energy dissipation in tanks with disk turbine and paddle agitators. The solid line corresponds to calculated results. Experimental data was taken from:

1 - Hixon, A.W. and S.J. Baum, Ind. Eng. Chem., 1942, v. 34, No. 1, p. 120.
2 - Barker, J. J. and R.E.Treybal, A.I.Ch.E. Journal, 1960, v. 6, No. 2, p. 289.
3 - Nikolaishvily, E. K., V.M.Barabash, L. N. Braginsky et al, *Theor. Found. of Chem. Eng.* (USSR), 1980, v.14, No.3, pp. 349-357 (USA translation - 1981).



ε energy dissipation
β mass transfer coefficient
ν kinematic viscosity of liquid
Sc Schmidt number, ν/D_{mol}
D_{mol} molecular diffusivity