

TITLE:

- Dataset underlying the research of: Fit parameters for liquid-solid fluidisation models applied in drinking water treatment processes

SHORT DESCRIPTION:

- In 2020 new accurate voidage prediction models were published in water treatment and multiphase flow related journal articles. The models were calibrated and validate for monodisperse spherical glass beads and fractionised calcite grains applied in water softening fluidised bed reactors. A spin off of this particular research project is that other granules also were examined, such as sand, steel and synthetic grains. The fit parameters for these grains were not shared with the scientific community. In short: this dataset consists of fit parameters for liquid-solid fluidisation models to predict the effective voidage applied in drinking water treatment processes and other multiphase flow systems in other industrial field for various granules, for various velocities, particle densities and temperatures.

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FORMAT:

- Numerical data

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ORGANIZATIONS:

- Delft University of Technology, Faculty of Civil Engineering and Geosciences, Department of Water Management
- Delft University of Technology, Faculty of Mechanical, Maritime and Materials Engineering, Department of Process and Energy
- Waternet, Amsterdam (funder)
- HU University of Applied Sciences Utrecht, Institute for Life Science and Chemistry

- Queen Mary University of London, Division of Chemical Engineering, School of Engineering and Materials Science

SUBJECT:

- Hydraulic modelling of multiphase flow systems

KEYWORDS:

- multiphase phenomena
- liquid-solid fluidisation
- drinking water treatment
- circular sustainable processes
- water softening
- model fit parameters

METHODOLOGICAL INFORMATION:

- Data set with fit parameters

ADDITIONAL TECHNICAL INFORMATION:

► O.J.I. Kramer, P.J. de Moel, J.T. Padding, E.T. Baars, Y.M.F. el Hasadi, E.S. Boek, J.P. van der Hoek, Accurate voidage prediction in fluidisation systems for full-scale drinking water pellet softening reactors using data driven models, *Journal of Water Process Engineering*. 37, 101481 (2020) 1–15. <https://doi.org/10.1016/j.jwpe.2020.101481>

► O.J.I. Kramer, J.T. Padding, W.H. van Vugt, P.J. de Moel, E.T. Baars, E.S. Boek, J.P. van der Hoek, Improvement of voidage prediction in liquid-solid fluidized beds by inclusion of the Froude number in effective drag relations, *International Journal of Multiphase Flow*. 127, 103261 (2020) 1–13. <https://doi.org/10.1016/j.ijmultiphaseflow.2020.103261>

2 Minimum and maximum fluidisation points

2.1 Minimum fluidisation points

Voidage prediction models are only valid for a fluidised state. For this reason, it is important to determine the incipient fluidisation point to check the prevailing state (Kramer et al., 2020a). The onset of fluidisation from fixed to fluidised state occurs when the drag force is equal to the weight of the particles and can be estimated using the very often used quadratic Equation (1), *e.g.* proposed by (Wen and Yu, 1966a) based on (Ergun, 1952). Although numerous prediction models are proposed in the literature, (Lippens and Mulder, 1993); (Anantharaman et al., 2018) there is no general agreement about the best approach. The degree of irregularity and polydispersity of particles as well as influences caused by the packing factor, surface forces, and wall effects increase the complexity of accurate prediction. For this reason, an established straightforward Wen–Yu method is chosen.

$$Re_{p,mf} = \sqrt{c_0^2 + c_1 Ar} - c_0 \quad (1)$$

And where $Re_{p,mf}$ is the incipient particle Reynolds number (Equation (2)) and Ar the Archimedes number (Equation (3)).

$$Re_{p,mf} = \frac{\rho_f v_{mf} d_p}{\eta} \quad (2)$$

$$Ar = \frac{g d_p^3 \rho_f (\rho_p - \rho_f)}{\eta^2} \quad (3)$$

In the literature (Yang, 2003) many values can be found for parameters c_1 and c_2 independent for the voidage at incipient fluidisation. The Wen–Yu Equation (1), based on the incipient particle Reynolds number $Re_{p,mf}$ and the Archimedes number Ar , were used to calculate the minimum fluidisation velocity. Fitting parameters for the Wen–Yu equation concerning spherical and natural were fitted through non-linear curve fitting and are given in Table 1.

Table 1 Model fit parameters (Equation (1))

Granule type	c_0	c_1	R^2
Reference			
(Wen and Yu, 1966a)	33.7	0.0408	n.a.
(Richardson and Zaki, 1979)	25.7	0.0365	n.a.
(Saxena and Vogel, 1977)	25.3	0.0571	n.a.
(Babu et al., 1978)	25.3	0.0651	n.a.
(Grace et al., 2020)	27.2	0.0408	n.a.
(Chitester et al., n.d.)	28.7	0.0494	n.a.
Spherical particles ²⁾			
Glass beads	29.3	0.0426	0.998
Steel shots	96.1	0.0613	0.999
Nylon balls	31.8	0.0442	0.984
Glass+steel+nylon	32.1	0.0444	0.997
Natural particles ²⁾			
Rapid filter sand	24.5	0.0423	0.953
Sand ¹⁾	38.2	0.0594	0.929
Calcite ²⁾			
Calcite pellets	24.6	0.0306	0.996
Crushed calcite	11.8	0.0271	0.898
Other particles ²⁾			
Zirconium balls	34.2	0.0429	0.998
Literature data ³⁾	177	0.0780	0.970

¹⁾ Rapid filter sand, garnet sand, crystal sand + (Đuriš *et al.*, 2016; Dharmarajah, 1982)

²⁾ Non-linear curve fit

³⁾ Sources: (Wilhelm and Kwauk, 1948; Lewis *et al.*, 1949; Richardson and Zaki, 1954; Loeffler, 1953; (Wen and Yu, 1966b); Dharmarajah, 1982; Hartman *et al.*, 1992; Đuriš *et al.*, 2016)

3 Data-driven model fit parameters

Note: Table 2, Table 3,

- 1) Rapid filter sand, garnet sand, crystal sand + ((Đuriš et al., 2016); (Dharmarajah, 1982)
- 2) 6.35 mm metal balls (Richardson and Zaki, 1954)
- 3) Sources: (Wilhelm and Kwauk, 1948); (Lewis et al., 1949); (Richardson and Zaki, 1954); (Loeffler, 1953); (Wen and Yu, 1966a); (Dharmarajah, 1982); (Hartman et al., 1992); (Đuriš et al., 2016)
- 4) $60 < v_s$ [m/h] < 120

3.1 Single Reynolds–Froude model (Rep1Frp)

Source: (Kramer et al., 2020b)

$$\varepsilon = c_0 Re_p^{c_1} Fr_p^{c_2} \quad (4)$$

Table 2 Model fit parameters (Equation (4))

Granule type	c_0	c_1	c_2	R^2
Spherical particles				
Glass beads	1.47	-0.0817	0.429	0.990
Steel shots	1.40	-0.0662	0.491	0.997
Nylon balls	1.87	-0.122	0.475	0.995
Glass+steel+nylon	1.52	-0.0870	0.438	0.988
Natural particles				
Crystal sand	2.29	-0.196	0.498	0.981
Garnet sand	2.01	-0.193	0.425	0.968
Rapid filter sand	1.87	-0.125	0.465	0.966
Sand ¹⁾	1.81	-0.132	0.422	0.934
Calcite				
Calcite pellets	1.64	-0.104	0.434	0.974
Crushed calcite	1.81	-0.135	0.393	0.979
Calcite pellets ⁴⁾	1.99	-0.168	0.444	0.986
Other particles				
Richardson–Zaki ²⁾	28.5	-0.422	0.844	0.995
Zirconium balls	1.19	-0.0849	0.331	0.965
Literature data ³⁾	1.68	-0.111	0.395	0.871

3.2 Double Reynolds–Froude model (Rep2Frp)

$$\varepsilon = (c_0 Re_p^{c_1} + c_2 Re_p^{c_3}) Fr_p^{c_4} \quad (5)$$

Table 3 Model fit parameters (Equation (5))

Granule type	c_0	c_1	c_2	c_3	c_4	R^2
Spherical particles						
Glass beads	1.46	-0.375	0.677	0.0261	0.459	0.994
Steel shots	57.6	-1.44	1.25	-0.0502	0.491	0.997
Nylon balls	141	-3.20	1.58	-0.0855	0.452	0.994
Glass+steel+nylon	1.34	-0.0621	1.08	-0.813	0.459	0.988
Natural particles						
Crystal sand	2.23	-0.188	0.600	-2.35	0.496	0.982
Garnet sand	1.96	-0.182	0.104	-0.877	0.435	0.969
Rapid filter sand	1.68	-0.341	0.563	0.0492	0.462	0.995
Sand ¹⁾	1.23	-0.0511	1.07	-0.538	0.465	0.992
Calcite						
Calcite pellets	1.69	-0.348	0.527	0.0575	0.456	0.994
Crushed calcite	1.62	-0.104	0.492	-0.917	0.400	0.981
Calcite pellets ⁴⁾	1.14	-0.0652	1.12	-0.445	0.464	0.993
Other particles						
Richardson–Zaki ²⁾	11.1	-0.518	5.43	-0.246	0.722	0.996
Zirconium balls	1.39	-0.369	0.382	0.0902	0.362	0.975
Literature data ³⁾	1.69	-0.260	0.375	0.0709	0.454	0.967

4 Reynolds-Froude numbers-based model fit parameters

4.1 Stokes–Oseen–Newton model (SON)

Source: (Kramer et al., 2020b)

$$f_T = \frac{c_0}{Re_\varepsilon} + \frac{c_1}{Fr_p} - c_2 \ln(Re_\varepsilon) + c_3 \quad (6)$$

Table 4 Model fit parameters (Equation (6))

Granule type	c_0	c_1	c_2	c_3	R^2
Spherical particles					
Glass beads	150	0.2313	0.1203	1.566	0.985
Steel shots	150	0.1975	0.1350	1.628	0.995
Nylon balls	150	0.2385	0.2193	2.422	0.997
Glass+steel+nylon	150	0.1509	0.1750	2.100	0.986
Natural particles					
Crystal sand	150	0.4556	0.6373	6.669	0.971
Garnet sand	150	0.5882	0.7685	2.301	0.778
Rapid filter sand	150	0.2257	0.1450	1.928	0.978
Sand ¹⁾	150	0.1463	0.2259	2.594	0.970
Calcite					
Calcite pellets	150	0.1597	0.2060	2.311	0.990
Crushed calcite	150	0.5005	0.3839	3.382	0.937
Calcite pellets ⁴⁾	150	0.1413	0.2307	2.636	0.970
Other particles					
Richardson–Zaki ²⁾	150	0.4587	0.6389	6.709	0.971
Zirconium balls	150	0.4139	0.4633	2.897	0.976
Literature data ³⁾	150	0.2274	0.1392	1.762	0.993

4.2 Reynolds–Improved–Outlook model (RIO1)

$$f_T = \frac{c_0}{RF} + \frac{c_1}{RF^{c_2}} \quad (7)$$

$$RF = Re_\varepsilon \frac{(1 + c_3 Fr_p^{c_4})}{(1 + c_5 Fr_p^{c_4})} \quad (8)$$

Table 5 Model fit parameters (Equation (7) and (8))

Granule type	c_0	c_1	c_2	c_3	c_4	c_5	R^2
Spherical particles							
Glass beads	150	10.95	11.91	0.4014	1.292	0.2353	0.991
Steel shots	150	5.487	196.3	21.71	4.376	0.1787	0.995
Nylon balls	150	16.14	55.56	14.63	2.194	0.3023	0.997
Glass+steel+nylon	150	12.38	11.26	0.1340	1.190	0.2578	0.987
Natural particles							
Crystal sand	150	2.195	10.45	52.51	4.129	0.1096	0.978
Garnet sand	150	5.658	66.33	7.773	3.577	0.05215	0.809
Rapid filter sand	150	4.574	6.986	0.1038	3.810	0.1590	0.976
Sand ¹⁾	150	5.152	14.72	7.668	6.532	0.1939	0.970
Calcite							
Calcite pellets	150	7.432	1.043	0.7184	1.128	0.2242	0.992
Crushed calcite	150	21.73	175.9	1.386	2.641	0.2191	0.949
Calcite pellets ⁴⁾	150	10.12	55.16	26.60	2.083	0.2731	0.942
Other particles							
Richardson–Zaki ²⁾	150	1.786	6.417	40.00	3.773	0.08462	0.970
Zirconium balls	150	2.853	2,903	9.563	5.963	0.08959	0.986
Literature data ³⁾	150	6.715	7.610	0.2733	1.972	0.1919	0.994

4.3 Reynolds–Improved–Outlook model (RIO2)

$$f_T = \frac{c_0}{RF} + \frac{c_1}{RFc_2} \quad (7)$$

$$RF = \left(Re_\varepsilon + c_3 Fr_p^{\frac{1}{c_2}} \right) \quad (9)$$

Table 6 Model fit parameters (Equation (7) and (9))

Granule type	c_0	c_1	c_2	c_3	R^2
Spherical particles					
Glass beads	150	5.157	4,816	0.1998	0.983
Steel shots	150	11.59	23,000	0.2915	0.993
Nylon balls	150	10.83	1,588	0.2936	0.997
Glass+steel+nylon	150	5.984	3,790	0.2192	0.986
Natural particles					
Crystal sand	150	7.374	113.8	0.2000	0.973
Garnet sand	150	32.13	7,249	0.3190	0.834
Rapid filter sand	150	5.453	1,981	0.1995	0.973
Sand ¹⁾	150	6.246	771.6	0.2263	0.970
Calcite					
Calcite pellets	150	6.703	2,052	0.2409	0.989
Crushed calcite	150	30.64	688.5	0.4225	0.935
Calcite pellets ⁴⁾	150	6.669	1,388	0.2604	0.900
Other particles					
Richardson–Zaki ²⁾	150	14.26	304.4	0.3000	0.971
Zirconium balls	150	5.039	48,780	0.2000	0.986
Literature data ³⁾	150	10.94	4,845	0.2842	0.989

4.4 Eureka symbolic regression model (EUR)

$$f_T = \frac{c_0}{Re_\varepsilon} + \frac{c_1}{\sqrt{Fr_p}} \quad (Re_\varepsilon < 15,000) \quad (10)$$

Table 7 Model fit parameters (Equation (7) and (10))

Granule type	c_0	c_1	R^2
Spherical particles			
Glass beads	150	0.8762	0.974
Steel shots	150	0.7193	0.981
Nylon balls	150	0.9457	0.972
Glass+steel+nylon	150	0.8722	0.976
Natural particles			
Crystal sand	150	1.503	0.954
Garnet sand	150	1.554	0.750
Rapid filter sand	150	1.023	0.968
Sand ¹⁾	150	1.030	0.958
Calcite			
Calcite pellets	150	0.9201	0.950
Crushed calcite	150	1.672	0.883
Calcite pellets ⁴⁾	150	0.9131	0.947
Other particles			
Richardson–Zaki ²⁾	150	1.503	0.954
Zirconium balls	150	0.6824	0.860
Literature data ³⁾	150	0.6982	0.944

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PROJECT:

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SHARING AND ACCESS INFORMATION:

- 4TU.ResearchData
- Delft, 7 January 2021