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Organic matter parameters in WWTP – a critical review and recommendations for application in activated sludge modelling

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ABSTRACT

This paper includes a comprehensive literature review of sludge composition data from wastewater treatment plants. 722 data sets from 249 sources were used to establish typical ratios between COD and solids-based parameters and to verify rule-of-thumb values, respectively. Confirmation of these typical ratios can also be accomplished by using biochemical composition data. It is shown that a correlation between data from proteins, lipids and carbohydrates analysis can be related to COD/VSS ratios. Finally, using the findings from the literature review, the organic and inorganic conversion factors of COD fractions in activated sludge models are adjusted to solids-based parameters. It was shown that with the adjustments of the factors and a partition of the particulate inert fraction into a fraction assigned to the influent and a fraction assigned to the endogenous products, a better agreement with the ratios of COD/VSS in the individual sludge streams can be established.

Key words: activated sludge modelling, chemical composition, COD characterization, organic solids, routine data, sludge composition, WWTP

HIGHLIGHTS

- Currently the largest collection of literature-based sludge data on municipal wastewater treatment plants.
- Recommendations for adjustment of specific VS contents in model fractions of activated sludge models and further model improvements.
- Linking biochemical data with typical wastewater parameters.

1. INTRODUCTION

In addition to its academic use, modelling of wastewater treatment plants (WWTPs) is a common task for engineers in practice, design and process control. While first model developments were based on volatile suspended solids (VSS) as a measure for biomass in activated sludge systems, Gujer & Jenkins (1975) introduced an oxygen equivalence in a universal modelling approach to get a balance for all processes related to organic matter. Finally, this resulted in the COD-based Activated Sludge Models (ASM) 1–3 (Henze *et al.* (1987), Henze *et al.* (1995), Henze *et al.* (1999), Gujer *et al.* (1999)).

For practical applications, a connection between the model fractions based on COD and the available routine data based on VSS or total suspended solids (TSS) is required. A widely used and accepted solution is the concept of observables, first introduced by Gujer & Larsen (1995). For every COD fraction in the model, a conversion factor is defined to calculate the TSS content of the fractions and the total solids content. This can also be calculated in relation to VSS.

On the other side, COD determination of activated sludge is not a common measure in routine data at WWTP due to problems regarding sample preparation and procedure. There are some rules of thumb for the link of COD and routine measures for organic matter in WWTP especially for the COD/VSS ratio. The most prominent value is 1.42 as the COD/VSS ratio for waste activated sludge (WAS) in a WWTP. This value is based on theoretical calculations with a chemical formula for biomass (Hoover & Porges (1952)) and is used in many publications and text books in our field.

By extension of a model to the complete WWTP including the sludge processing units there are other types of sludge of interest, mainly

- primary sludge (PS),
- mixed (raw) primary and waste activated sludge before anaerobic digestion (RS) and
- anaerobic digested sludge (ADS).

For these sludge types reliable COD/VSS ratios are missing, therefore one of the main aims of this paper is the review and definition of reasonable values, in order to enable COD-based WWTP modelling using typically available measurements for total and volatile solids. An additional theoretical examination is established as a base for verification of the review results.

Another aim is to combine this data with information from biochemical families; for example, protein lipid and carbohydrate content. Due to a variety of thematic overlaps, this appears to be a useful addition; for example, in order to be able to compare data from the fermentation of biological residues and waste materials.

Finally, a comparison of the current practice of linking COD-based data from activated sludge modeling with operational data from wastewater treatment plants based on TS or VS is provided. It is investigated to what extent the currently used conversion factors are suitable to accurately describe the actual conditions.

2. THEORETICAL CONSIDERATIONS

For every substance the molecular mass and also the COD can be calculated based on chemical fundamentals. Since these substances are of organic origin, the mass corresponds to volatile mass and the COD/VSS ratio can be calculated when the chemical composition of organic matter is known.

$$C_nH_aO_bN_c + \left(n + \frac{a}{4} - \frac{b}{2} - \frac{3}{4}c\right)O_2 \rightarrow nCO_2 + \left(\frac{a}{2} - \frac{3}{2}c\right)H_2O + cNH_3 \quad (1)$$

Equation (1) can be used to calculate COD of any organic substance consisting of carbon, oxygen, hydrogen and nitrogen.

Wastewater (WW) and different types of sludge in WWTPs consist mostly of organic matter with regard to carbon content. The organic carbon content can be divided into the following 3 major groups:

- Lipids (from fat, oil and grease)
- Proteins (from biomass) and
- Carbohydrates (organic waste, residues, cell walls etc.)

Other minor and exotic fractions exist (e.g. amino sugars, lignin, alcohols, volatile organic compounds, etc.) but their influence will only be important in certain cases, which would require a more sophisticated approach anyway.

The smallest possible fat is a triglyceride with butyric acid and the elemental formula $C_{15}H_{26}O_6$ (Tributyrin, PubChem CID 6050). Typical fats consist of fatty acids with chain lengths of more than 3 carbon atoms. Most animal or plant-based fats have chain-lengths in the range of 10–20 (Rustan & Drevon (2005)). Some example calculations can be found in Table 1. From the COD/VSS range of components of lipids, a high value for the complete lipid molecule can be expected. With increasing chain length of fatty acids (more than 10), the COD/VSS ratio results in values larger than 2.5. Therefore, values from Pöpel (1975/88) seem to be quite low but are used by many researchers in further work. Sometimes also values for single fatty acids were used in literature (e.g. Barker & Stuckey (1999), Grady *et al.* (2011)) to calculate soluble microbial products. Own calculations based on the fatty acid composition of 20 randomly selected edible fats and oils (see Reeves & Weihrauch 1979) result in a typical value of 2.88 g COD/g VSS (Effenberger & Kühn 2018).

Proteins are typically composed of 22 different canonical amino acids (AA). Literature gives information about the distribution of these different AA in bacterial, eukaryotic and archaean proteins (e.g. Kozlowski (2016), Cañizares-Villanueva *et al.* (1995)). The peptide bonds of multiple AA are formed by condensation reactions, which produce one water molecule per bond. This reaction reduces VSS but does not alter COD. From about 20–30 AA upwards, the change in the COD/VSS ratio by additional bonds is negligible. This effect increases the COD/VSS ratio of a long protein chain of a certain AA by about 16% in comparison to a single AA. Mean size for bacterial protein is about 300 amino acids (Tiessen *et al.* (2012)).

Table 1 | Stoichiometric calculations of COD/VSS ratio for different substances and organisms

Compound	Chemical formula	Molar weight =VSS [g/Mole]	Required oxygen = COD [Mole O_2]	[g/Mole]	COD/VSS	Source	Remarks
Biomass							
Biomass (general)	$C_5H_7O_2N$	113.1	5.0	160.0	1.414	Hoover & Porges (1952), also cited by Irvine & Bryers (1985)	Alternative $CH_{1.4}O_{0.4}N_{0.2}$
Biomass	$C_8H_{14}O_4N$	188.2	8.8	280.0	1.488	Pitter & Chudoba (1990)	Activated sludge
Biomass	$C_{118}H_{170}O_{57}N_{17}P$	2,738.7	119.3	3,815.8	1.393	Sawyer (1956)	Activated sludge
Biomass	n.d.				1.2–1.66	Bullock *et al.* (1996)	Own experiments from activated sludge
Biomass	n.d.				1.16–1.29	Contreras *et al.* (2002)	Own experiments from activated sludge
Biomass	n.d.				1.15–1.57	Friedrich & Takács (2013)	Model-based determination of own experiments
Pure bacterial culture	Variable				1.14–1.49	Roels (1983)	
Pure bacterial culture	$C_6H_{10}O_3N$	144.1	6.3	200.0	1.387	Pitter & Chudoba (1990)	
Escherichia coli	$CH_{1.69}O_{0.58}N_{0.2}$	25.8	1.0	31.4	1.219	Folsom & Carlson (2015)	Under diff. limiting conditions
Escherichia coli	$CH_{1.71}O_{0.37}N_{0.24}$	23.0	1.1	34.0	1.477	Folsom & Carlson (2015)	Under diff. limiting conditions
Algal biomass	$C_{106}H_{263}O_{110}N_{16}$	3,522.2	104.8	3,351.8	0.952	Stumm & Morgan (2012)	Alternative $CH_{2.48}O_{1.04}N_{0.15}$
Picking beans (*Phaseolus vulgaris*)	$CH_{1.81}O_{0.81}N_{0.15}$	28.9	0.9	29.9	1.035	Pineda-Insuasti *et al.* (2014)	
Oyster mushroom (*Pleurotus ostreatus*)	$CH_{1.83}O_{0.84}N_{0.26}$	30.9	0.8	27.0	0.871	Pineda-Insuasti *et al.* (2014)	
Sawdust	$CH_{1.19}O_{0.59}N_{0.007}$	22.7	1.0	31.9	1.403	Buragohain *et al.* (2010)	
Rice husk	$CH_{1.7}O_{0.83}N_{0.003}$	27.0	1.0	32.2	1.192	Buragohain *et al.* (2010)	
Bamboo dust	$CH_{1.66}O_{0.9}N_{0.018}$	28.3	1.0	30.4	1.074	Buragohain *et al.* (2010)	
Lignin	$(C_9H_{9.45}O_{2.65})_n$	159.9	10.0	321.2	2.009	Effenberger & Kühn (2018)	Based on Freudenberg (1965)
Components of lipids							
Glycerin	$C_3H_8O_3$	92.1	3.5	112.0	1.216		Base compound of lipids
Butyric acid	C_3H_7COOH	88.1	5.0	160.0	1.816	PubChem 264	Simplest fatty acid
Butyric acid lipid	$C_{15}H_{26}O_6$	302.4	18.5	592.0	1.958	PubChem 6050	Simplest fat
Decanoic acid	$C_9H_{19}COOH$	172.3	14.0	448.0	2.600	PubChem 2969	Animal and herbal lipids
Palmitic acid	$C_{15}H_{31}COOH$	256.4	23.0	736.0	2.870	PubChem 985	Animal and herbal lipids
Eicosapentaenoic acid	$C_{19}H_{29}COOH$	302.5	26.5	847.9	2.804	PubChem 446284	Omega-3 fatty acid
Hexacosanoic acid	$C_{25}H_{51}COOH$	396.7	38.0	1,215.9	3.065	PubChem 10469	Animal or herbal wax
Carbohydrates							
Glucose	$C_6H_{12}O_6$	180.2	6.0	192.0	1.066		Basic component of all polysaccharides

(*Continued*)

Table 1 | Continued

Compound	Chemical formula	Molar weight =VSS [g/Mole]	Required oxygen = COD [Mole O_2]	[g/Mole]	COD/VSS	Source	Remarks
Starch	$C_{12}H_{22}O_{11}$	342.3	12.0	384.0	1.122	PubChem 439341	Metabolic product
Glycogen	$C_{24}H_{42}O_{21}$	666.6	24.0	768.0	1.152	PubChem 439177	Metabolic product
Typical compositions							
Organic matter	$C_{18}H_{19}O_9N$	393.3	17.5	560.0	1.424	Henze *et al.* (2002)	Orig. source Pöpel (1975/88)
Organic matter in domestic WW	$C_{10}H_{19}O_3N$	201.3	12.5	400.0	1.987	Grady *et al.* (2011)	
Lipids	$C_8H_6O_2$	134.1	8.5	272.0	2.028	Pöpel (1975/88)	
	$C_8H_6O_2$	134.1	8.5	272.0	2.028	Henze *et al.* (2002)	Orig. source Pöpel (1975/88)
	$C_8H_6O_2$	134.1	8.5	272.0	2.028	Sophonsiri & Morgenroth (2004)	Orig. source Henze *et al.* (2002)
	no formula				2.91	Miron *et al.* (2000)	Orig. source Sayed (1987)
	$C_{50}H_{90}O_6$	787.3	69.5	2,223.9	2.825	Alves *et al.* (2009)	
	$C_{54.9}H_{99.8}O_{6.0}$	854.6	76.9	2,459.2	2.878	Effenberger & Kühn (2018)	Based on 20 random edible fats and oils
Grease	$C_8H_{16}O$	128.2	11.5	368.0	2.870	Grady *et al.* (2011)	
Carbohydrates	$C_5H_9O_{4.5}$	141.1	5.00	160.0	1.134	Pöpel (1975/88)	
	$C_{10}H_{18}O_9$	282.2	10.0	320.0	1.134	Henze *et al.* (2002)	Orig. source Pöpel (1975/88)
	$C_{10}H_{18}O_9$	282.2	10.0	320.0	1.134	Sophonsiri & Morgenroth (2004)	Orig. source Henze *et al.* (2002)
	$C_6H_{12}O_6$	180.2	6.0	192.0	1.066	Miron *et al.* (2000)	Also used as CH_2O by many authors
	$C_6H_{10}O_5$	162.1	6.0	192.0	1.184	Alves *et al.* (2009)	
	$(C_{11.2}H_{17.8}O_{9.5})_n$	304.2	10.9	348.8	1.147	Effenberger & Kühn (2018)	Mix of various carbohydrates
Proteins	$C_7H_6O_{3.5}N$	160.1	6.0	192.0	1.199	Pöpel (1975/88)	
	$C_{14}H_{12}O_7N_2$	320.3	12.0	384.0	1.199	Henze *et al.* (2002)	Orig. source Pöpel (1975/88)
	$C_{14}H_{12}O_7N_2$	320.3	12.0	384.0	1.199	Sophonsiri & Morgenroth (2004)	Orig. source Henze *et al.* (2002)
	$C_4H_{6.1}O_{1.2}N$	87.4	4.2	133.6	1.529	Miron *et al.* (2000)	Orig. source Sanders *et al.* (1996)
	$C_4H_{6.1}O_{1.2}N$	87.4	4.2	133.6	1.529	Mahmoud *et al.* (2004)	Orig. source O'Rourke (1968)
	$C_{16}H_{24}O_5N_4$	352.4	16.5	528.0	1.498	Alves *et al.* (2009)	Identical to Grady *et al.* (2011)
	$C_{16}H_{24}O_5N_4$	352.4	16.5	528.0	1.498	Grady *et al.* (2011)	
	$C_{4.37}H_{6.85}N_{1.26}O_{1.38}S_{0.03}$	99.97	4.5	144.2	1.447	Effenberger & Kühn (2018)	Based on food amino acid composition, see Sosulski & Imafidon (1990)

Distribution of canonical AA in archaea, bacteria and eukaryotes can be found in literature (e.g. Cañizares-Villanueva *et al.* (1995), Kozlowski (2016)). With that distribution and the calculated COD of included AA, a mean chemical composition can be derived to $C_{6.8}H_{13.2}O_{2.9}N_{1.7}$. This leads to a COD/VSS ratio of 1.44, which is in the range of literature values from Table 1. Own calculations based on the amino acid composition of 23 foods presented by Sosulski & Imafidon (1990) result in a similar ratio (Effenberger & Kühn 2018).

Carbohydrates are biological molecules consisting of carbon, oxygen and hydrogen. They can be divided depending on their degree of polymerization into sugars, oligosaccharides and polysaccharides. Their chemical composition can be described with formula $C_m(H_2O)_n$. They play a major role in growth of all kinds of life. Some examples can be found in Table 1.

Based on the chemical composition of these 3 groups of WW and sludge components, their mass resp. VSS content (under assumption of solid state of aggregation) and their COD content regarding Equation (1) can be calculated, resulting in a COD/VSS ratio. Table 1 shows some principal examples. Amino acids can be found separately in the supplementary material.

By mixing of these different component properties regarding COD and VSS of most types of WW and sludge can be described.

From these theoretical considerations the following ranges of COD/VSS ratio can be derived:

- lipids >2 – typically 2.9
- proteins 1.4–1.5
- carbohydrates 1.07–1.18

3. REVIEW OF LITERATURE DATA OF WWTP SLUDGE

3.1. Literature survey

There are a large number of publications related to sludge of WWTP. Most of them contain data regarding the composition and different measures of the type of sludge under investigation. In the course of research, 249 different publications were found containing suitable data sets ($n=722$). The search for suitable sources was carried out via the database Web of Science (http://isiknowledge.com). Using various keywords and combinations, sources were identified and then manually screened. Furthermore, sources related to these sources were evaluated (forward and backward citation). Through this step-by-step but also time-consuming procedure, a very large number of sources could be found without, however, achieving completeness. This lack is compensated by the number of sources and data sets included.

The following criteria has to be fulfilled to include a dataset into evaluation:

- measures for COD, solids and volatile solids content
- description of origin
- type of sludge

The following additional parameters were recorded when they were presented in the paper:

- information about sludge composition (esp. content of lipids, proteins and carbohydrates)
- additional remarks regarding prior treatment, composition and blending

During data processing it has been shown that it is useful to define four different types of sludge:

- Primary sludge PS:
  sludge from primary clarifiers or waste activated sludge from WWTP with low sludge retention times (SRT<10 days)
- Waste activated sludge WAS:
  sludge from WWTP with sufficient SRT (>10 days)
- Mixed PS and WAS (PS+WAS):
  mixed raw sludge before anaerobic digestion or other sludge treatment
- Anaerobic digested sludge (ADS):
  mesophilic or thermophilic digested sludge

Some datasets show properties from another type of sludge as defined by the author, often a sludge was classified as WAS but the properties suggest that it is actually PS. These datasets were not manually eliminated or reattributed to another type of sludge. Aditionally, the possibility that published data is biased towards more exotic cases (e.g. industrial wastewater with high concentrations of lipids or carbohydrates), may potentially result in a shift of the ratios.

Furthermore there are some special types of sludges and substrates included in the database for comparison.

3.2. Measures related to total and volatile organic matter

The analysis of COD as well as solids content is broken down into different fractions depending on the purpose. In the present case, the COD/VSS ratio is sought, whereby the particulate COD is required more precisely, since it is a matter of characterizing sludge mass flows. These consist of a high proportion of particles. However, hydrolysis can convert particulate compounds to dissolved fractions given the appropriate residence time, so using the total COD may also be useful. This applies analogously to TS and VS.

In general, solids analysis can be systematized according to Figure 1. By knowing TS, TSS, VS and VSS, all missing quantities can be calculated.

These four analytical parameters are also found in various literature sources evaluated. The inorganic fractions are essentially determined by the site-specific boundary conditions (flushing of solids from the surface, salinity of the discharged wastewater). At the same time, the salinity of a typical drinking water or wastewater, for example, can also be estimated from empirical values. Thus, verifications of the equation system from Figure 1 are possible and the quality of individual analyses can be evaluated.

From a practical point of view, it should be noted that sample filtration can only be reasonably carried out up to a certain limit of solids content. Thus, it can be roughly estimated that all sludges (PS, WAS) occurring on the wastewater side of a sewage treatment plant as well as the wastewater itself can still be filtered comparatively well. However, as soon as further thickening or dewatering has been carried out, only a determination of TS and VS or the conceivable use of a dilution method are practical. Both lead to the expectation of various error influences. This also applies to the determination of the dissolved COD content.

With regard to sludge streams of WWTPs, the dissolved components typically play a minor role because the particulate fractions dominate due to the high solids concentrations. Hence, for municipal wastewater treatment, the concentration differences between TS and TSS or VS and VSS are generally considered within the margin of error, if TSS concentrations are larger than 20–30 g/l.

3.3. Sludge composition based on biochemical families

In addition to data on sludge composition with regard to COD and solids, the publications examined in some cases also contained information on sludge composition related to biochemical families of lipids, proteins and carbohydrates (LPC). Due to the direct relation to the material composition, these parameters are therefore also considered.

However, the research revealed a very wide variety in terms of the analytical methods and calculations used. This makes a comparative evaluation enormously difficult. For example, in some of the sources, a direct analysis of the three components was carried out, while in other sources only two of the components were measured in the laboratory and the missing one was

		Filtered sample		Filter residue
TS	=	TDS	+	TSS
=		=		=
(T)VS	=	VDS	+	VSS
+		+		+
(T)FS	=	FDS	+	FSS

Figure 1 | Different types of solids measures ((TS, total solids; TDS, total dissolved solids; TSS, total suspended solids; (T)VS, (total) volatile solids; VDS, volatile dissolved solids (organic dissolved matter, organic molecules and salts); VSS, volatile suspended solids (organic particulate matter, biomass); (TFS), (total) fixed (or non-volatile) solids; FDS, fixed dissolved solids (inorganic matter, salts); FSS, fixed suspended solids (inorganic particulate matter)).

determined by difference formation. Both VS and COD were used as reference values. Furthermore, various conversions of LPC data into COD based on VS can be found in the literature.

A standard method for the determination of lipid content has existed for many years (APHA (2017)). However, there are various other analytical methods in the literature, some of which are based on the standard methods.

With regard to protein analysis, a comparison of the analytical methods used has already been carried out by various authors and for different substances studied. Frølund *et al.* (1996) and Raunkjær *et al.* (1994) have each compared methods for the analysis of proteins and carbohydrates. While Frølund *et al.* (1996) determined similar accuracies of the two methods considered for carbohydrates, Raunkjær *et al.* (1994) were able to demonstrate very large differences with respect to accuracy.

Similarly divergent results were obtained from the individual investigations in regard to protein content. Jimenez *et al.* (2013) have taken up these investigations and carried out their own comparisons for protein and carbohydrate analysis specifically based on colorimetric methods. However, in the conclusions it is recommended to choose the appropriate method depending on the application and the investigated substrate matrix, as there is obviously no universally best analytical method.

In addition to the different analytical methods, the LPC values in the studied sources were also presented with different references. Two main groups are found: Reference to the organic solids (VS or VSS) or reference to COD.

To ensure comparability, component specific conversion factors were obtained. Two different sources were found (see Table 2 for results). The conversion factor of 2.91 g COD/g lipids used by Miron *et al.* (2000) was taken from a dissertation on slaughterhouse wastewater (Sayed (1987)), but in this work it is merely quoted from another currently unavailable source in the field of meat processing. However, the conversion factor of 1.15 g COD/g protein also used from Sayed (1987) from another unavailable source in the form of conference proceedings is not used by Miron *et al.* (2000). Instead, a value of 1.50 g COD/g protein based on another unavailable conference proceedings article is used (Sanders *et al.* (1996)). This value is also used by Mahmoud *et al.* (2004), but cited from a much older source (O'Rourke (1968)). However, a recalculation using the chemical formula for protein by Miron *et al.* (2000) gives a factor of 1.53 g COD/g protein.

Sophonsiri & Morgenroth (2004) use conversion factors based on stoichiometric calculations with molecular formulas for LPC from Henze *et al.* (2002). These, in turn, are based on publications by Pöpel (1975/88) without explaining the exact methodology behind the published chemical molecular formulas. The chemical formulas used by the various authors are also included in Table 1. By analyzing the authors or citations involved in each source, it is noticeable that the sources Miron *et al.* (2000) and Mahmoud *et al.* (2004) including the cited sources Sayed (1987) and Sanders *et al.* (1996) are closely related. This is analogously true for the publications of Sophonsiri & Morgenroth (2004) with Henze *et al.* (2002) and Pöpel (1975/88). Such correlations can also be examined very well on a larger scale with a bibliometric analysis (Ahnert & Krebs (2021)).

For an exemplary test of these two data sets with conversion factors (Table 2)), data from Mahmoud *et al.* (2004) were used (Table 3). The calculation shows a very good agreement for the factors according to Miron, while the other set of conversion factors gives a very large underestimation of the COD.

The conversion factors recommended by Miron *et al.* (2000) agree very well with the calculated values from the chemical formulas for LPC of Alves *et al.* (2009) (see also Table 1), although further explanation of the formulas is unfortunately missing.

4. RESULTS AND DISCUSSION OF THEORETICAL AND REVIEW RESULTS

4.1. Solids

The evaluation of the investigated data regarding the different solid measurements is summarized in the form of ratio values in Table 4.

Table 2 | Different sets of conversion factors from VSS VS into COD [g COD/g LPC]

Lipids	Proteins	Carbohydrates	Source
2.03	1.20	1.13	Sophonsiri & Morgenroth (2004)
2.91	1.50[a]	1.07	Miron *et al.* (2000)

[a]Correct value of 1.53 for complete oxidation reaction of $C_4H_{6.1}O_{1.2}N$.

Table 3 | COD calculation based on LPC data with different sets of conversion factors

	Total	Sol.	Part.		Miron factors[a]	Sophonsiri factors	
Protein	6.22	0.07	6.15	g/L	9.40	7.38	g COD/L
Lipids	6.50		6.50	g/L	18.92	13.20	g COD/L
Carbohydrates	1.33	0.06	1.33	g/L	1.42	1.50	g COD/L
Sum	14.05		13.98	g/L	**29.74**	**22.08**	g COD/L
VS	14.72			g/L			
TS	20.35			g/L			
COD	30.00	1.92	**28.07**	g/L	**5.9%**	**−21.4%**	deviation

[a]With correct value of 1.53.

Table 4 | Descriptive statistics for relations of solids concentrations from literature

TSS/TS	PS	WAS	PS+WAS	ADS	*VSS/VS*	PS	WAS	PS+WAS	ADS
n	8	27	33	9	**n**	8	21	26	9
Mean	0.87	0.85	0.83	0.90	**Mean**	0.89	0.93	0.86	0.91
Median	**0.88**	**0.88**	**0.85**	**0.92**	**Median**	**0.90**	**0.93**	**0.88**	**0.92**
SD	0.10	0.11	0.11	0.04	**SD**	0.05	0.06	0.08	0.03
RSD	11.3%	12.3%	13.8%	4.7%	**RSD**	5.6%	6.5%	9.3%	3.3%
Max	0.99	0.97	0.96	0.94	**Max**	0.96	0.99	0.98	0.95
Min	0.65	0.55	0.60	0.81	**Min**	0.81	0.78	0.69	0.86
VSS/TSS	PS	WAS	PS+WAS	ADS	*VS/TS*	PS	WAS	PS+WAS	ADS
n	52	90	37	58	**n**	57	120	89	71
Mean	0.75	0.75	0.74	0.67	**Mean**	0.71	0.73	0.73	0.62
Median	**0.76**	**0.74**	**0.76**	**0.68**	**Median**	**0.73**	**0.74**	**0.75**	**0.63**
SD	0.11	0.08	0.08	0.10	**SD**	0.12	0.10	0.09	0.11
RSD	15.2%	11.0%	11.2%	14.5%	**RSD**	16.9%	13.3%	11.6%	18.1%
Max	0.96	0.89	0.86	0.81	**Max**	0.90	0.96	0.86	0.87
Min	0.37	0.54	0.42	0.36	**Min**	0.38	0.35	0.43	0.21

A subdivision was made into the four defined sludge types. The number of evaluated data pairs for TSS/TS and VSS/VS is significantly lower compared to the ratio values VSS/TSS and VS/TS. The scatter in the form of standard deviation SD or relative standard deviation RSD is very low for all four investigated ratios and all sludge types. Surprising is the generally very high number of suspended solids measurements (both VSS and TSS), since it is to be expected that a filtration of these sludges is difficult to perform.

A statistical test for differences in the mean values was performed for all ratio values examined (ANOVA, p=0.01). This revealed statistically significant differences between the different sludge types for VSS/TSS and VS/TS. These differences are also to be expected due to the different formation or treatment of the sludge types.

The difference between analyses for total solids and suspended solids is the respective salinity or organic dissolved compounds. Peng *et al.* (2020) indicate a TDS content in artificial industrial wastewater (WW) of 3.4–12.1 g/L, real municipal WW was analyzed with a TDS of 0.8 g/L. According to WHO & IPCS (1996) dissolved solids affect the taste of drinking water (good between 0.3 and 0.6 g/L, unacceptable >1.2 g/L).

Therefore, a calculation of the TSS/TS ratio was made with the following assumptions. A data series was generated from a water with a TDS content of 1 and 2 g/L, respectively. This already corresponds to a very saline wastewater. Then total solids (meaning organic solids) were mathematically added to this water up to a TS concentration of 100 g/L. The results are shown as solid lines in Figure 2.

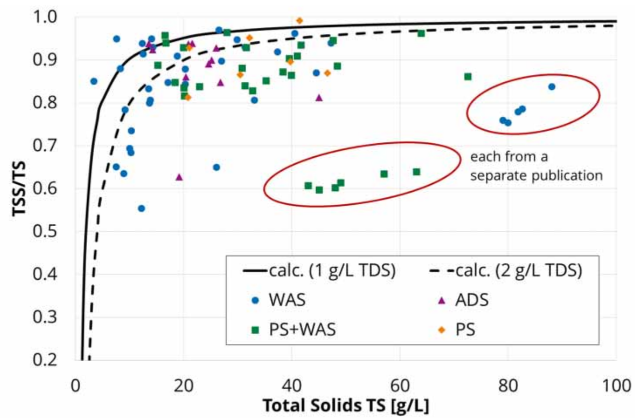

Figure 2 | Theoretical prediction and data from literature survey for TSS/TS ratio.

All available data pairs with TS and TSS values from the literature research were also plotted on the graph depending on the sludge type. It is expected that the data points are in the range of the theoretical calculations. As can be easily seen from Figure 2, this is rather inadequately true for a large number of data points. Data from two publications (outlined in red) show a massive deviation, suggesting systematic errors in the analytics or extremely high TDS concentrations (e.g. influence of brackish or saline water). It can be concluded for a large number of the existing data sets that obviously the TSS is underestimated because the TS analytics is generally simple in its execution and thus the underestimation of the TSS/TS ratio is caused by TSS, particularly at higher TSS concentrations. However, since the relevant statements of this paper are aimed at the COD/VSS ratio, the influence on these values nevertheless seems to be rather small (although it cannot be excluded that similar problems are present in the VSS/VS ratio, but cannot be tested in the same way).

4.2. COD and COD/VSS ratio

The results of the statistical evaluation with respect to COD in the form of the ratio CODs/CODt (dissolved/total COD) are shown in Table 5. It can be clearly seen that there is a large scatter in the ratio. The reasons for this can be manifold, such as different pretreatment procedures, storage and residence times, sampling techniques, and so on. Overall, however, the dissolved fraction is very low at less than 10% of total COD. Nevertheless, for a consideration of the particulate COD, the dissolved fraction should be subtracted from the total COD in order to avoid the error influence in this respect.

The COD to organic dry matter ratios for the four sludge types are shown as distributions in Figure 3. A distinction is made between four different ratios: CODt/VS, CODt/VSS, CODp/VS, CODp/VSS with CODp (particulate)=CODt-CODs. Since the present work is intended to characterize the properties of sludge streams, it is obvious to relate these values to CODp. In order not to wrongly consider dissolved solid relevant compounds, a reference to VSS would be the logical consequence. However, knowing the possible problems with the analysis of suspended solids in higher concentration ranges (see previous chapter), the use of the VS as a reference value also seems reasonable.

Table 5 | Statistical data of ratio of dissolved and total COD in different samples from literature survey

CODs/CODt	**PS**	**WAS**	**PS+WAS**	**ADS**
n	77	147	60	90
Mean	0.07	0.03	0.08	0.06
Median	**0.05**	**0.02**	**0.07**	**0.03**
SD	0.04	0.03	0.05	0.06
RSD	57.1%	100.0%	62.5%	100.0%
Max	0.25	0.18	0.20	0.36
Min	0.01	0.00	0.00	0.00

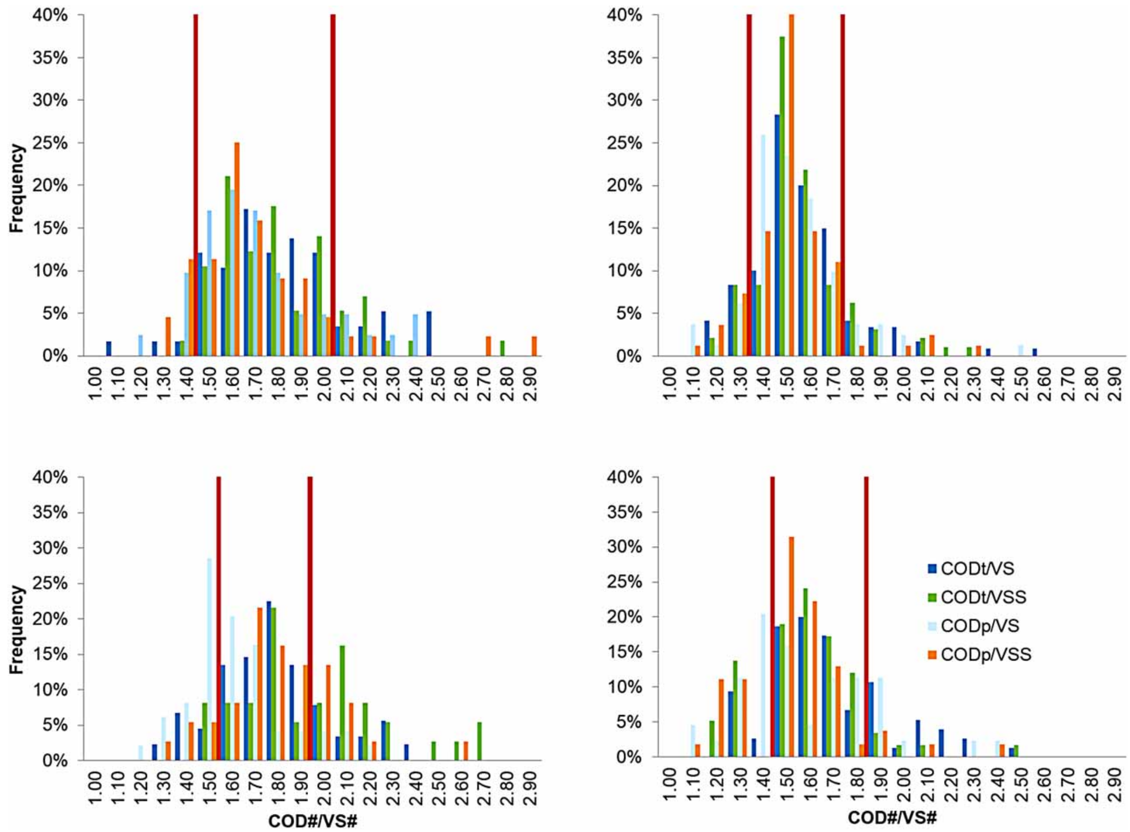

Figure 3 | Distribution of different COD/VS ratios for different sludge types (red bars show lower and upper boundaries regarding to calculations in Table 7). The full colour version of this figure is available in the online version of this paper, at http://dx.doi.org/10.2166/wst.2021.419.

For basic plausibility reasons, all statistically determined values for the individual sludge types with respect to COD#/VS# ratios were limited downward to 1.07 (carbohydrates) and upward to 3 (lipids) based on the theoretical considerations in Chapter 2. Data sets outside these limits were not considered in the evaluation.

From the plots in Figure 3, a generally existing normal distribution can be seen for all four sludge types. There is a tendency for some values to be found in larger value ranges, so that a slight skewness in the distributions can be recognized. Since an overestimation of COD is unlikely, problems in the determination of the organic solids content could have caused these unusually high ratio values.

The statistical data of the representations from Figure 3 are summarized in Table 6. While PS and PS+WAS show a small scatter, this is somewhat more pronounced for WAS and ADS, but still in a rather small range. There tend to be higher mean values compared to the median. Due to the large number of data sets, this suggests possible outliers in the high value range, as already deduced from the representation of the distribution. Therefore, the use of the median values is preferred at this point.

A significance test for differences in means (ANOVA, $p=0.05$) of the various ratio values as a function of sludge types reveals no significant differences, although the values obviously differ.

The higher median values for WAS, PS+WAS and ADS between CODp/VS and CODp/VSS are striking. Since VSS must always be smaller than VS, this can be explained. The ratio values based on the total COD are also higher than the respective values with reference to CODp according to the dissolved fraction included. Combining this with the effect from VSS/VS leads to the largest values.

It is also noticeable that the PS+WAS yields larger ratio values than would be expected from a mixture of the values of PS and WAS. A plausible cause could not be deduced from the data. However, there are a variety of factors influencing the composition of the mixture of PS and WAS, such as mixing ratios, inputs in the catchment area, pretreatments, residence times in previous treatment stages, etc.

Table 6 | Statistical data of different COD/VS ratios from literature survey

		CODt/ VS	CODt/ VSS	CODp/ VS	CODp/ VSS		CODt/ VS	CODt/ VSS	CODp/ VS	CODp/ VSS
PS	**N**	58	58	41	44	**WAS**	120	96	81	82
	Mean	1.77	1.79	1.68	1.66		1.53	1.52	1.49	1.48
	median	1.74	1.73	1.63	1.58		1.50	1.49	1.44	1.45
	SD	0.29	0.30	0.27	0.30		0.22	0.19	0.21	0.19
	RSD	16.4%	16.8%	16.1%	18.1%		14.4%	12.5%	14.1%	12.8%
	Max	2.50	2.94	2.39	2.81		2.55	2.29	2.50	2.24
	Min	1.09	1.39	1.16	1.28		1.11	1.11	1.08	1.08
PS+WAS	**N**	89	37	49	37	**ADS**	75	58	44	54
	Mean	1.75	1.91	1.56	1.76		1.66	1.55	1.54	1.48
	Median	1.74	1.81	1.52	1.74		1.60	1.55	1.46	1.48
	SD	0.25	0.31	0.21	0.25		0.26	0.22	0.28	0.23
	RSD	14.3%	16.2%	13.5%	14.2%		15.7%	14.2%	18.2%	15.5%
	Max	2.33	2.62	2.15	2.52		2.40	2.40	2.36	2.39
	Min	1.25	1.41	1.15	1.22		1.26	1.13	1.08	1.10

For further considerations and comparisons, the median values of the CODp/VSS ratio are used, because these correspond most closely to the aspect under investigation.

4.3. Connection between LPC and COD/VSS ratio

The LPC data obtained in the literature data evaluation were processed and partially converted to evaluate the relative proportions related to the respective sludge types. The results are summarized in Table 7.

In contrast to the COD/VSS ratios, the significantly larger fluctuation range is recognizable. Reasons for this can be seen not only in the natural fluctuation in the composition but also in the different analytics. Other influencing factors such as the

Table 7 | Relative content of LPC from literature survey in different sludge types

rel. lipid content	PS	WAS	PS+WAS	ADS	rel. carbo-hydrates cont.	PS	WAS	PS+WAS	ADS
n	7	31	11	8	**n**	7	31	11	8
Mean	0.22	0.05	0.18	0.13	**Mean**	0.45	0.21	0.36	0.32
Median	0.26	0.03	0.16	0.16	**Median**	0.46	0.16	0.35	0.33
SD	0.11	0.05	0.04	0.05	**SD**	0.13	0.13	0.08	0.14
RSD	48%	94%	22%	40%	**RSD**	29%	60%	22%	45%
Max	0.36	0.17	0.30	0.19	**Max**	0.63	0.61	0.50	0.52
Min	0.09	0.01	0.16	0.04	**Min**	0.21	0.07	0.20	0.09
rel. protein content	**PS**	**WAS**	**PS+WAS**	**ADS**	**calc. COD/VSS[a][g COD g VSS^{-1}]**	**PS**	**WAS**	**PS+WAS**	**ADS**
n	7	31	11	8					
mean	0.32	0.74	0.45	0.55	**Mean**	1.63	1.51	1.62	1.57
median	0.30	0.80	0.45	0.50	**Median**	1.68	1.49	1.58	1.59
SD	0.09	0.15	0.08	0.13	**Max**	1.93	1.73	1.85	1.75
RSD	29%	21%	17%	24%	**Min**	1.37	1.26	1.51	1.35
max	0.48	0.91	0.59	0.83	**Median CODp/VSS from Table 6:**				
min	0.23	0.33	0.34	0.43	**CODp/VSS**	1.58	1.45	1.74	1.48

[a]With corrected conversion factors from Table 2. Max value: max. lipid content, min. carbohydrates content. Min value: min. lipid content, max. carbohydrates content.

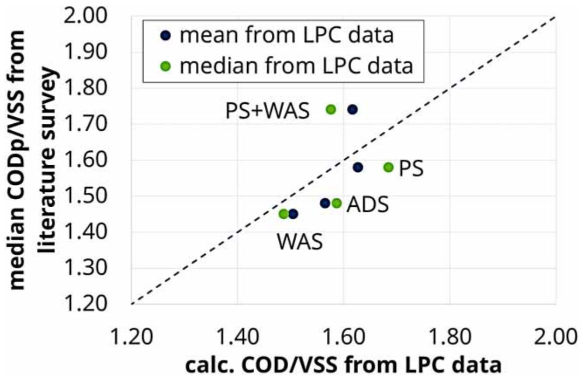

Figure 4 | Comparison of CODp/VSS ratio from literature and calculated from LPC data.

type of pretreatment or the composition of the treated wastewater are also conceivable. Using the factors according to Miron (Table 2), the CODp/VSS ratios for the four sludge types were calculated from the mean and median value of LPC data. A comparison of the ratios calculated in this way with the data from the literature research is shown in Figure 4.

It can be seen very well that it is largely consistent between both methods (the dashed line represents the expected value). Depending on the use of the mean or median value of the LPC data, there are still shifts, which are relatively large for PS and PS+WAS. However, it can be stated at this point that basic ratios of the CODp/VSS ratio can also be derived from LPC data. The comparatively large deviations for PS+WAS can be attributed to the small database and strongly fluctuating lipid contents depending on the catchment area.

In the lower right area of Table 7, a lower and upper limit of the COD/VSS ratio was calculated from the statistically determined LPC data. For this purpose, the maximum lipid content and the minimum carbohydrate content were combined for the maximum values and the minimum lipid content and the maximum carbohydrate content were combined for the minimum values. In each case, missing balance fractions were assumed to be protein.

The limits thus determined were plotted as red bars in Figure 3 to visualize a plausible range. While PS and PS+WAS show a strong range of variation due to the influent-specific properties, a much narrower distribution can be seen for WAS and ADS.

This can also be derived in a similar form from Figure 5. There, the calculated total COD values based on the LPC data with the conversion factors from Table 2 are compared with the actual analysis values. It can be seen that there is an underestimation of about 5% (Miron factors) and 20% (Sophonsiri factors). One reason for the general underestimation could be that there is obviously an underestimation of proteins or lipids, which leads to lower calculated COD values. However, the Miron factors already represent a good approximation, as discussed above.

5. APPLICATION TO PLANT-WIDE-MODELLING

5.1. Solids in activated sludge models

The practical application of the CODp/VSS ratio arises in the dynamic simulation of wastewater treatment plants with an activated sludge model. These are based on the COD as a balancing variable. However, many measurements from plant practice and operating data are available as TS or VS, especially when sludge and solids-relevant material flows are involved. As described in the introduction, this concept of conversion was introduced into activated sludge modeling by Gujer & Larsen (1995).

All ASMs published to date, starting with ASM 2, contain corresponding fraction-specific conversion factors (see Table 8). An adjustment of these ratios according to the practical data and experience from the above literature analyses has not yet been demonstrated in the literature.

The origin of these factors cannot at present be directly and unambiguously assigned. A situation clearly deviating from each other in time is apparent. While the three activated sludge models listed contain identical parameters (at least related to TSS), later publications contain different (mostly higher values) for the COD/VSS ratio. This is especially true for particulate biodegradable organic matter XS. In addition, a distinction between non-biodegradable organic matter from influent (XI, Inf) and from endogenous biomass (XP or XI) has been made in the later publications, which corresponds better to reality

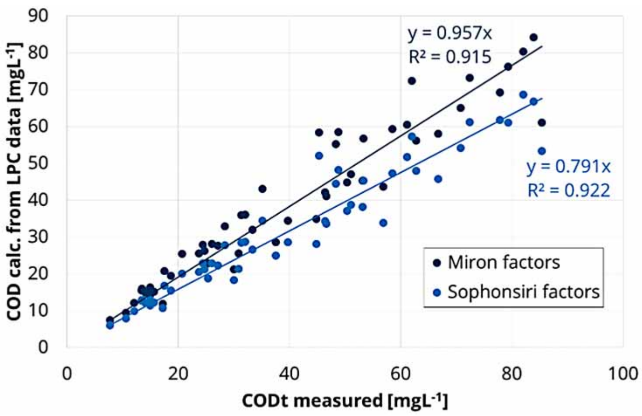

Figure 5 | Correlation between measured and calculated total COD based on LPC data.

Table 8 | Models and sources with specific TS or VS contents of major model fractions (terminology based on ASMs)

italics – calculated			**iTSS or iVSS (depending on unit)**					**COD/VSS or COD/TSS**					
Model	**Source**	**Units**	**XI,Inf**	**XP (XI prod.)**	**XS**	**BM**	**XSTO**	**XI**	**XP**	**XS**	**BM**	**XSTO**	**Remarks**
ASM2	Henze *et al.* (1995)	g TSS (g COD)$^{-1}$	0.75		0.75	0.90		*1.33*		*1.33*	*1.11*		
ASM2d	Henze *et al.* (1999)	g TSS (g COD)$^{-1}$	0.75		0.75	0.90		*1.33*		*1.33*	*1.11*		
ASM3	Gujer *et al.* (1999)	g TSS (g COD)$^{-1}$	0.75		0.75	0.90		*1.33*		*1.33*	*1.11*		
		g VSS (g COD)$^{-1}$	0.75		0.75	0.75		*1.33*		*1.33*	*1.33*		
Barker & Dold model	Barker & Dold (1997)	g TSS (g COD)$^{-1}$				*0.68*					1.48		Non-polyP het. BM
		g TSS (g COD)$^{-1}$				*0.70*					1.42		polyP het. BM
ASM3+bioP	Rieger *et al.* (2001)	g TSS (g COD)$^{-1}$	0.75		0.75	0.90	0.60	*1.33*		*1.33*	*1.11*	*1.67*	
ASM2d+TUD	Meijer (2004)	g TSS (g COD)$^{-1}$	0.75		0.75	0.90	0.60	*1.33*		*1.33*	*1.11*	*1.67*	
BioWin	EnviroSim (2016)	g VSS (g COD)$^{-1}$	*0.63*	*0.70*	*0.63*	*0.70*		1.60	1.42	1.60	1.42		
SumoC	Dynamita (2020)	g VSS (g COD)$^{-1}$	*0.77*	*0.70*	*0.56*	*0.70*	*0.60*	1.30	1.42	1.80	1.42	1.67	
	Labelle *et al.* (2017)	g VSS (g COD)$^{-1}$	*0.63*	*0.68*	*0.57*	*0.70*		1.60	1.48	1.74	1.42		
	Alikhani *et al.* (2017)	g VSS (g COD)$^{-1}$	*0.67–0.50*	*0.70*	*0.56*	*0.70*		1.50–2.00	1.42	1.80	1.42		From diff. sources
	Yang *et al.* (2019)	g VSS (g COD)$^{-1}$	*0.67*	*0.77*	*0.56*	*0.70*		1.50	1.30	1.80	1.42		From diff. sources

and also enables a distinction to be made in model terms between non-degradable matter from the influent and from the process itself.

5.2. Organic and inorganic solids

For a correct differentiation between organic and total dry matter, the consideration of the inorganic fraction in the COD fractions is of interest. This is generally also referred to as ash content, since in solids analysis the residue remaining after incineration corresponds to the inorganic content. Table 9 compiles various data on ash contents from different bacteria or general biomass based on elemental analyses rather than incineration.

While in some of the listed models (Table 8) the conversion of COD fractions into TSS is given (although probably VSS is rather meant), starting with the ASM3 as well as in some current approaches a correct distinction is made between TSS and VSS. In the ASM3, the inorganic fraction in a fraction (biomass) was explicitly shown for the first time by the difference between the two factors for VSS and TSS. However, all other fractions did not contain inorganic TSS (ISS). During endogenous decay of biomass, the ISS contained therein is then released and thus assigned to the corresponding fraction. No explanation is given for this approach.

In Grady *et al.* (2011), the ash content of biomass is given as 15% (based on dry mass). When determining ash content, it should be noted that the difference between organic and total dry mass alone results in an increase in mass due to oxidation or carbonation of the contained metals. Estimates with data of the bacterial metallome from various sources (in Table 9) have shown a calculated increase in mass of the inorganic fraction of 50–100%, if complete oxidation or carbonation is assumed. Thus, it can be assumed that the value given by Grady *et al.* (2011) was calculated using a difference method from solid analysis.

This is certainly true for the calculable inorganic solids fraction (ISS) considered in ASM3 (see Table 8). The difference 0.90 g TSS g COD^{-1}–0.75 g VSS g COD^{-1} results in 0.15 g ISS g COD^{-1} assuming ISS = TSS – VSS.

Wentzel *et al.* (2002) reports 0.17 mg ISS mg VSS^{-1} for biomass (0.119 g ISS g COD^{-1} assuming 1.42 g COD g VSS^{-1} for biomass) and inert endogenous decay products XI, while inert particulate COD XI,Inf in the influent has no ISS fraction.

Ekama & Wentzel (2004b) used data from a wide variety of experimental and real plants to develop a steady state model to describe the ISS balance and determine 0.15 mg ISS mg VSS^{-1} for biomass (0.106 g ISS g COD^{-1}). In reference to Ekama & Wentzel (2004a), no ISS was assigned to the inert endogenous products XI. The reason given is the composition of ISS from cell-internal TDS and the unformulated assumption that all cell contents are immediately released when cells die. This conclusion cannot be followed and it is recommended, also for logical reasons, to assign the same ISS content to XI as to biomass. In the ISS model of Ekama & Wentzel (2004b), ISS accumulates in a WWTP from influent (0.05 g ISS g COD^{-1} for raw and 0.035 g ISS g COD^{-1} for primary treated WW) and from uptake of TDS during biomass growth.

Table 9 | Ash content of different types of bacteria

Source	Species	Remarks	Ash content
Barton *et al.* (2007)	*Desulfovibrio desulfuricans*	Anaerobic sulfate-reducing bacteria	6.4%
Todar (2015)	General composition		8.8%
Ho *et al.* (2003)	General composition		9.2%
Scherer *et al.* (1983)	*M. bryantii*	Euryarchaeote methane producing archaea	10.5%
	M. arboriphilus	Most fundamental species of the genus Methanosarcina	16.3%
	Methanobact. spec.		11.0%
	M. mazei		11.3%
	Methanosarcina	Anaerobic archaea	5.5%
	M. barkeri 1		6.4%
	M. barkeri 2		7.3%
	M. barkeri 3		7.2%
Cordier *et al.* (1987)	*E. coli*		7.5%
	Methylophilus methylotrophus	Aerobic bacteria	6.2%
	K. fragitis (substrate lactose)	Yeast	7.2%
	K. fragitis (substrate galactose)		7.8%
	K. fragitis (substrate glucose)	Anaerobic sulfate-reducing bacteria	6.5%

5.3. COD influent characterization

In the DWA rules for the design of single-stage wastewater treatment plants (DWA-A-131 (2016)) as well as in an internationally oriented adaptation of these design rules for wastewater treatment plants in other climate regions (Expoval (2019)), a fractionation of the COD is carried out as in the activated sludge models.

The simulation with activated sludge models in the typical application areas with respect to temperature and SRT and using the available fractionation experience in the influent again results in typical compositions of the resulting sludges with respect to the COD/VSS ratio.

For the characterization of COD in the influent of a wastewater treatment plant or in the effluent of the primary clarification, there are different fractionation methods in practical use (e.g. Roeleveld & van Loosdrecht (2002), Melcer (2004), Expoval (2019) based on DWA-A-131 (2016)). These methods give general ranges of COD fractions in the influent of a wastewater treatment plant. At the same development, results of region-specific fractionations and their summaries can be found in various sources (e.g. Yang *et al.* (2019)).

As an example, some value ranges can be found in Table 10. It should be noted that for activated sludge models, the influent characterization of heterotrophic biomass is used as a workaround to integrate another slowly degradable component. For historical reasons, it made sense to limit the model fractions because of computational time, so this workaround was used, knowing well that there is not as much active biomass in the influent. However, compared to the biomass stored in an activated sludge plant with sufficiently large SRT, this is an acceptable simplification.

5.4. Adaptation of research results and discussion

The presented findings from the literature research are now analyzed in a simulation scenario for their effect regarding the COD/VSS ratio. For this purpose, the software Simba#4.3 (ifak (2021)) was used to build a wastewater treatment plant model based on ASM3 (Gujer *et al.* (1999)) with the parameter set according to Koch *et al.* (2000) and a few modifications according to Alex *et al.* (2007). In addition, in the ASM, a division of fraction XI into XI,Inf as well as XI (from endogenous products) was made for balancing reasons, as it is already implemented in some activated sludge models (e.g. Hu *et al.* (2007)). The restriction to only one inert particulate fraction was historically done to limit the computational effort.

The WWTP itself was designed for nutrient removal with upstream denitrification and simultaneous chemical phosphorus precipitation according to DWA-A-131 (2016). The influent loading of the model was done statically with the design input data. The plant has a primary treatment with 1 h HRT (based on the model according to Otterpohl & Freund (1992)) and is operated with a SRT of 15 d. Based on the value ranges in Table 10, the following parameters of the influent fractionation and the wastewater temperature were varied or combined:

- SI = 0.05 * COD
- SS = 0.2 * COD
- XI,inf = (0.1–[0.02] - 0.2) * COD
- XH = (0.1–[0.02] - 0.2) * COD
- WW temperature = 10–[2] – 20 °C

Table 10 | COD influent characterization for raw municipal wastewater

	Soluble		Particulate (colloidal)		
	Non biodeg. SI	Readily biodeg. SS	Slowly biodeg. XS	Non biodeg. XI	Het. biomass XH
Henze & Comeau (2008)	0.03–0.08	0.05–0.26	0.47–0.53	0.13	0.10
Roeleveld & van Loosdrecht (2002)	0.04–0.10	0.11–0.42	0.10–0.47	0.23–0.50	–
Alex *et al.* (2007) based on DWA-A-131 (2016)	0.05–0.10	0.10–0.40[a]	Remaining part of balance	0.10–0.20	0.18[a]

[a]From biodegradable COD.

Both soluble parameters were fixed because they have no direct influence on CODp/VSS ratio. In any case, the model fraction SS is converted to XH via XSTO. A variation between SS and XS therefore only requires the additional hydrolysis step to produce SS from XS. The fraction of COD in the influent that is allocated to the fraction XS results from the balance. The total of 216 simulations were evaluated for the three sludge types PS, WAS and PS+WAS.

The conversion factors from Table 11 were used for comparison. These were used to calculate the CODp/VSS ratios for the three sludge types PS, WAS and PS+WAS. It is again pointed out that these calculations have no influence on the simulation results themselves but are subsequently calculated from the simulation results using fraction-specific conversion factors (observables concept from Gujer & Larsen (1995)). When using a controller to adjust the solids concentration in the activated sludge tank based on measured values of MLSS or MLVSS, these actually conservative variables, i.e. not involved in the processes, then become active in the model and directly influence the conversion performance.

The three sludge types differ significantly in their composition with respect to the COD fractions (Figure 6 left). PS consists of about 50% slowly biodegradable substrate. Regardless of the name, this fraction contains both particulate and colloidal components. This is reflected, for example, in a reduced settling effect in the model of the primary clarifier. Furthermore, PS is composed of inert particulate matter and biomass. The latter, however, as already explained, is only a workaround to create an additional fraction for slowly biodegradable matter.

WAS is primarily composed of biomass (about 47%). The other fractions are about half inert particulate matter from influent XI,infl and formed inert particulate matter from endogenous respiration. Both XS and XSTO are present only in minor proportions because the activated sludge has largely converted these compounds by sufficient SRT.

The mixture of PS and WAS then roughly results in a three-way split into biomass, XS and inert particulate matter.

A conversion of the COD fractions from the simulated 216 scenarios to VSS is shown in Figure 6 (right). The unfilled bars correspond to the distribution for the three sludge types with the standard conversion factors. The resulting mean values for PS (1.56), WAS (1.39), and PS+WAS (1.47) are lower than the values from the literature search (Table 6). Using the standard

Table 11 | Standard and modified parameter sets for conversion factors from COD to VSS and resulting CODp/VSS ratios

	iVSS,#		CODp/VSS	
	Standard	**Modif.**	**Standard**	**Modif.**
XI,inf	0.752	**0.625**	1.33	***1.6***
XI	0.752	**0.704**	1.33	***1.42***
XS	0.556	0.556	1.8	1.8
XBM	0.704	0.704	1.42	1.42
XSTO	0.600	0.600	1.67	1.67

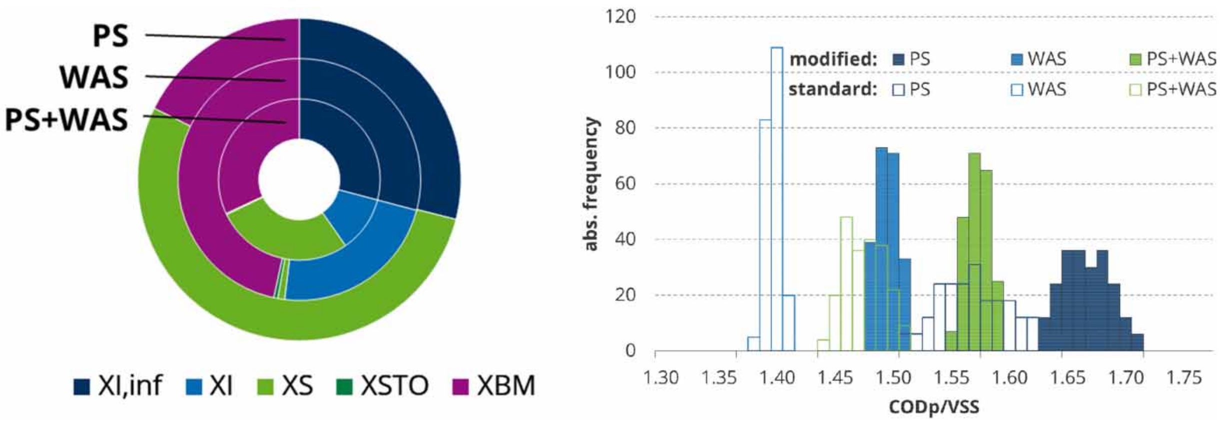

Figure 6 | Left: Proportions of the model fractions in the sludge types; right: distribution of CODp/VSS ratios for sludge types and different sets of conversion factors.

conversion factors in the context of plant-wide modeling in comparison with operating data, which are mostly available on a TS or VS basis, results in underestimates of the sludge flows produced in the model. This makes model adjustment more difficult or leads to misinterpretations. Therefore, an adjustment of the conversion factors is necessary. As shown in Table 8, there are already various adjustment approaches.

In order to raise the CODp/VSS ratio into the desired range, the following procedure was chosen (results under modified in Table 11).

WAS: The factor for biomass conversion is generally accepted (Table 1) and is therefore left as it is. Noticeable is the changed factor for biomass decay and the resulting endogenous products. Therefore, an adjustment analogous to various other sources was made (Table 8). The last fraction that remains to be adjusted is XI,inf. Since the COD/VSS ratio in the influent tends to be high in general, an adjusted value of 1.6 g COD/ g VSS is chosen. This then places WAS in the typical range of Table 6 as well as from various sources.

For PS, improvements already result from adjusting XI,Inf and XI from the WAS adjustment.

The resulting CODp/VSS ratios with the modified conversion factors according to Table 11 are 1.66 (PS), 1.49 (WAS) and 1.57 (PS+WAS) and are thus in the range of the data from the literature evaluations (Table 6).

By increasing the COD/VSS ratio, the chemical energy stored as COD is assigned to a lower mass of VSS, so the energy density increases. At the same time, lower solids contents in the model result for the same conversion processes. If a model correction is made with above adjustments to operating solids content data, a slightly higher sludge age must be set to achieve the same solids content. Thus, the previous conversions would have contained a lower level of confidence.

However, the resulting changes are in a small range. Comparing the parameters from Table 11, the reductions of the VSS mass calculated from the COD are 5.8% (PS), 6.6% (WAS) and 6.2% (PS+WAS) compared to the standard conversion factors. A change in ISS content from 0.15 g ISS g COD^{-1} (ASM3) to 0.106 (Ekama & Wentzel (2004b)) - 0.12 (Wentzel *et al.* (2002)) g ISS g COD^{-1} results in decreases in TSS content of 4.3–6.7% depending on sludge type and conversion factor. Thus, the effects are within the range of analytical uncertainties.

With these adjustments (which do not mean any modification of the model itself), a very good agreement of the CODp/VSS ratios can be established for a use in interaction with operational data of wastewater treatment plants. Therefore, it is recommended to extend the activated sludge model with respect to inert particulate fractions for practice-relevant simulation calculations. This is feasible with little effort and without expected cross-influences. As an advantage, a greater freedom arises with regard to the adjustment with operating data. The present work further leads to the conclusion that, for correct implementation, a separation of the fraction of slowly biodegradable matter into a particulate and a colloidal fraction should also be carried out (compare e.g. Hauduc *et al.* (2018)), which should be examined right away in combination with a change of the usual practice of the approach of heterotrophic biomass in the influent for balance reasons. However, the resulting impacts within an activated sludge model are estimated to be much more complex and therefore cannot be discussed within the scope of this paper.

Furthermore, the effect of conversion adjustments on anaerobically stabilized sludge (ADS) was not tested in terms of modeling. This requires the use of an appropriate anaerobic model and evaluation of the conversion factors contained therein, or alternatively, a simplified digestion model based on the existing ASM fractions. This is also outside the scope of this paper and should still be considered in further research.

6. CONCLUSIONS

The explanations given in this paper span an arc from a large data set of information from a variety of literature sources on the composition of sludge, to the possibilities and limitations of linking various variables from monitoring and modeling of wastewater treatment plants, to application in the context of practice-relevant simulation calculations.

With the data set and the statistical parameters from Table 6, experiences and rule of thumb values have been proven with sufficient certainty. At the same time, these values can be used for the evaluation of own sludge analyses in order to carry out a case study in case of strong deviations from these characteristic data.

Furthermore, it is possible to link chemically determined wastewater parameters such as COD with biochemical parameters such as protein, lipid and carbohydrate content.

The application of the findings from the literature review leads to a modified set of conversion factors for the calculation of solids-based variables in the context of activated sludge modeling. This allows a better linkage of the simulation calculations with practically used parameters. As indicated by the researched conversion factors and the discussion, more attention should be paid to this aspect of modeling in order to clarify the presented uncertainties regarding organic and inorganic conversion factors in the future and to seek a consistent approach.

DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

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