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MOUSE

Biological Processes

Reference Manual

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MOUSE BIOLOGICAL PROCESSES

Reference Manual

1 Introduction

The MOUSE Biological Processes (BP) module simulates the reaction processes in multi-compound systems. The BP module solves the system of differential equations describing physical and biological interactions involved in the survival of bacteria and oxygen conditions in sewers.

Organic matter is modelled either on the basis of BOD or COD input (which is optional for the user) and a global converting factor between BOD and COD. The BOD/COD - DO relations are described as aerobic processes only, and BOD/COD degradation is omitted in the model when simulating anaerobic conditions.

The processes and concentrations of the modelled components are influenced by modelled temperature, flow velocities, sedimentation and re-suspension rates. Therefore, the MOUSE BP module is integrated with both the AD module and the ST module. E.g., as a basis for the description of the water quality conditions, the AD module calculates the water temperature.

The following pollution components are possible to include in the module:

Dissolved oxygen DO
Dissolved BOD/COD BOD_{dis}
Suspended BOD/COD BOD_{susp}
Faecale coli bacteria $COLI_f$
Total coli bacteria $COLI_t$
Streptocci bacteria STREP
Dissolved ammonia NH4
Dissolved phosphorus PO4

When modelling BOD/COD as a PPC component, e.g. modelling of sediment-attached BOD based on the use of Pollutant Partitioning Coefficients, BOD_{susp} is divided into two fractions - fine and coarse. Both fractions are modelled as isolated suspended components using the same set of equations and parameters.

Dissolved ammonia and phosphorus are modelled as a conservative transport using the AD module only, e.g. no biological processes are included. NH4 and PO4 can be modelled as PPC's.

2   BOD/COD - DO Interactions

The interaction between organic matter and oxygen in sewers are based on following principle:

BOD/COD is degraded both in the water phase and in the biofilm attached to the sewer pipe using two different principles in the calculation of the BOD/COD reduction.

In the water phase, the heterotrophic biomass is generated by growth on readily biodegradable substrate and the process is normally described as:

$$BOD_{degra} = K_s \cdot \theta^{temp-20} \cdot (BOD)/(BOD + k_{m,BOD}) \cdot (DO)/(DO + k_{m,DO}) \cdot B_x \qquad (2.1)$$

where:

K_s	=	μ_{max}/Y_{max} (Max growth rate at 20°C / Max yield constant),
q	=	temperature constant,
$k_{m,BOD}$	=	half-saturation constant, BOD dissolved,
$k_{m,DO}$	=	half-saturation constant, DO,
B_x	=	biomass of active heterotrophic organisms.

The suspended heterotrophic organisms are responsible for the degradation of dissolved BOD/COD in the water phase. In order to use Equation (2.1), the biomass of the heterotrophic microorganisms B_x in the system must be known.

In MOUSE BP it is assumed that the heterotopic biomass constitutes a certain fixed fraction of the suspended BOD/COD (0.5-1.0). Consequently, the degradation of dissolved BOD/COD by this group of micro-organisms is modelled by using a fixed fraction of the suspended BOD/COD as the biomass and apply this estimated biomass to Equation (2.1).

For the biofilm, it is assumed that there exists a thick biofilm in the sewer pipe, and that oxygen is the limiting factor for the degradation of dissolved BOD/COD. This means that the diffusion rate of DO from the water phase into the biofilm determines the degradation rate of dissolved BOD/COD in the biofilm attached to the sediment and the pipe

Hydrolysis of suspended BOD/COD converts the suspended material into dissolved substrate. This process can be modelled as a temperature-dependent 1st order reaction (Henze et al. 1986). Suspended BOD/COD is produced in sewers due to the growth of heterotrophic organisms. This process can be modelled by applying a yield constant to the degradation rate for dissolved BOD/COD in the water phase. The model is shown is Figure 2.1.
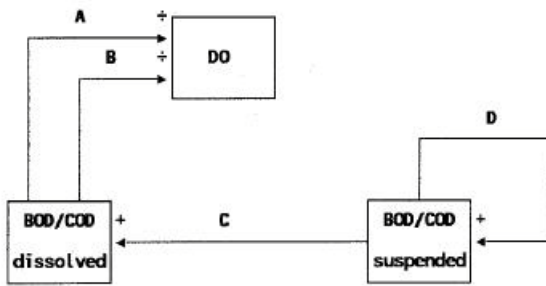
Figure 2.1   Conceptual diagram of the BOD/COD-DO model. Process A is degradation in biofilm, process B is degradation in water phase, process C is hydrolysis and process D is growth of heterotrophics

3 Oxygen Processes

A number of processes affect the oxygen concentration:

3.1 Re-aeration

Re-aeration is modelled in pipes only if they are not full flowing. The re-aeration equation is based on the difference between the actual and the saturation concentration of DO coupled to the hydraulic conditions /6/.

$$REAR = k1 \cdot (1 + k2 \cdot u^2 / (g \cdot d_m)) \cdot (s \cdot u)^{k3} \cdot d_m^{-1} \cdot (C_s - DO) \qquad (3.1)$$

where:

k1, k2, k3	= re-aeration parameters,
u	= flow velocity (m/s),
g	= gravitation (m/s²),
dm	= hydraulic mean depth (m),
Cs	= oxygen saturation concentration (g DO/m³).

The oxygen saturation concentration C_s is temperature-dependent and is calculated by means of a standard equation:

$$C_s = 14.652 + T \cdot (-0.41022 + T \cdot (0.007991 - 0.000077774 \cdot T)) \qquad (3.2)$$

where *T* is the water temperature (°C).

3.2 Degradation of BOD$_{dis}$ in Biofilm

The degradation of dissolved BOD/COD in biofilm is described as a standard ½-order reaction combined with a temperature-dependent oxygen diffusion and removal:

$$BOD_{degra, biofilm} = \theta^{temp - 20} \cdot \sqrt{2D} \cdot k_{of} \cdot DO^{\frac{1}{2}} \cdot A_{biofilm} / V \qquad (3.3)$$

where:

θ	=	temperature coefficient,
D	=	diffusion coefficient of oxygen in water at 20°C (m²/s),
k_{of}	=	removal of oxygen in biofilm at 20°C (g DO/m³·s),
$A_{biofilm}$	=	area in pipe covered with biofilm (=water) (m²),
V	=	water volume (m³).

The value of *D* is 20.0 (Jensen 1983, Gujer&Boller 1990) and *kof* has been measured to 3.0 (Andreasen 1979, Arvin&Harremoës 1990).

Notice: Degradation of BOD_{dis} in biofilm is activated only if oxygen consumption in biofilm is modelled!

3.3 Degradation of BOD_{dis} in Suspension

The degradation of dissolved BOD/COD carried out by suspended heterotrophics is described as:

$$BOD_{degra,\,susp} = K_s \cdot \Theta^{temp-20} \cdot BOD / (BOD + k_{m,\,BOD}) \qquad (3.4)$$
$$\cdot\, DO / (DO + k_{m,\,DO}) \cdot k_b \cdot BOD_{susp}$$

where:

Ks	=	μ_{max}/Y_{max} (day^{-1}) (Max growth rate at 20°C / Max yield constant),
θ	=	temperature coefficient,
km,BOD	=	half-saturation constant, BOD dissolved (g/m^3),
km,DO	=	half-saturation constant, DO (g/m^3),
kb	=	fraction of active heterotrophic organism in BOD_{susp}.

According to litterature, μ_{max} varies from 3.0 to 13.2 day^{-1} and $Ymax$ varies from 0.6 to 0.7 kg VSS/kg BOD (Henze et al .1986). The values for Km,BOD and km,DO are by default set to 8 g BOD/m^3 and 2 g DO/m^3 , respectively (Henze et al .1986, Arvin & Harremoës 1990). kb varies from 0.5 to 1.0.

3.4 Hydrolysis of BOD_{susp}

Hydrolysis of suspended matter is described as a temperature-dependent 1st order reaction:

$$BOD_{hydro} = \Theta^{temp-20} \cdot k_{hl} \cdot BOD_{susp} \qquad (3.5)$$

where:

Θ	=	temperature coefficient,
k_{hl}	=	1st order decay constant at 20°C (day^{-1}).

The value of k_{hl} is in the range of 0.05 - 0.10 day^{-1}.

3.5 Growth of Heterotrophics (BOD_{susp})

The growth of heterotrophics is dependent of the BOD degradation in the water phase, and the equation reads:

$$BOD_{growth} = Y_{max} \cdot BOD_{degra,\,susp} \qquad (3.6)$$

3.6 Eroded Sediment Oxygen Demand

When modelling ST and BP simultaneously, eroded sediment will cause an immediate oxygen consumption. The oxygen decrease is depending of the amount of sediment eroded and its oxygen demand. The eroded sediment oxygen demand is described as:

$$SED_{oxdemand} = k_{sed} \cdot SED_{eroded} \cdot 1/(V \cdot dt) \qquad (3.7)$$

where:

$ksed$	= oxygen demand of sediment (g DO/ m^3 sediment),
$SEDeroded$	= amount of eroded sediment in timestep (m^3 sediment),
V	= water volumen (m^3),
dt	= timestep (days).

Notice: Eroded sediment oxygen demand is activated only when ST and BP are modelled simultaneously.

3.7 Oxygen Balance (DO)

The differential equation describing the effects of these processes on the dissolved oxygen concentration reads:

$$dDO/dt = REAR - BOD_{degra, biofilm} - BOD_{degra, susp} - SED_{oxdemand} \qquad (3.8)$$

3.8 Dissolved BOD/COD Balance (BOD$_{dis}$)

The balance for BOD$_{dis}$ is:

$$dBOD_{dis}/dt = BOD_{hydro} - BOD_{degra, biofilm} - BOD_{degra, susp} \qquad (3.9)$$

3.9 Suspended BOD/COD Balance (BOD$_{susp}$)

The differential equation for BOD$_{susp}$ reads:

$$dBOD_{susp}/dt = BOD_{growth} - BOD_{hydro} \qquad (3.10)$$

4 Decay of Bacteria

Most pathogenic microorganisms are usually unable to multiply or survive for extensive periods in the aquatic environment. Eschericia coli (E. coli) is one of the dominant species in faeces from human and warm-blooded animals. The organism itself is normally considered non-pathogenic, but is very often used as indicator for faecal pollution and hence a potential for the presence of real pathogenic microorganisms.

In the MOUSE BP model, two methodologically defined groups of coliforms are distinguished: "Total coliform" and " Faecal coliform". The concept "Total coliform" may include a wide range of bacterial genera of which many are not specific of faecal contamination. Further more a third group of bacteria is included in the model - Streptocci bacteria.

The three groups of bacteria are modelled in the water phase with a temperature-dependent 1st order decay rate.

4.1 Decay Rate for Faecal Coliform (COLI$_{f,decay}$)

$$COLI_{f,\,decay} = \Theta^{temp-20} \cdot k_f \cdot COLI_f \tag{4.1}$$

where:

θ =   temperature coefficient,

kf =   1st order decay constant at 20°C (day^{-1}).

The value of k_f is in the range of 0.6 - 0.8 day^{-1}.

4.2 Decay Rate for Total Coliform (COLI$_{t,decay}$)

$$COLI_{t,\,decay} = \Theta^{temp-20} \cdot k_t \cdot COLI_t \tag{4.2}$$

where:

θ =   temperature coefficient,

kt =   1st order decay constant at 20°C (day^{-1}).

The value of kt is in the range of 0.7 - 0.9 day^{-1}.

4.3 Decay Rate for Streptoccoci (STREP$_{decay}$):

$$STREP_{decay} = \Theta^{temp-20} \cdot k_s \cdot STREP \tag{4.3}$$

where:

θ = temperature coefficient,

ks = 1st order decay constant at 20°C (day^{-1}).

The value of ks is in the range of 0.5 - 1.0 day^{-1}.

5   Pollutant Partitioning Concept (PPC)

The behaviour of sediments and sediment-attached pollutants is modelled in MOUSE by coupling the BP and the ST modules. This is achieved by attaching pollutants to two sediment fractions in terms of mass of pollutants per volume of sediment. The concept for modelling sediment-attached pollutants has been derived by Crabtree et al. (1993).

MOUSE operates with three sediment types and two fractions: surface sediments, pipe sediments, and foul flow sediments, a fine and a coarse fraction.

Surface sediments and pipe sediments are considered to consist of two fractions, a coarse mineral fraction comprised of particles > 0.5 mm (D50 = 1 mm) and a fine mineral fraction comprised of particles < 0.5 (D50 = 0.1 mm). Both the fine and the coarse mineral fractions are assumed to have the same density which is 2650 kg/m^3.

Foul flow sediments are assumed to consist only of a fine sediment fraction which is primarily organic. The density of this fraction is approximately 1800 kg/m^3.

In MOUSE, pollutants are modelled both as dissolved and sediment-attached. The modelling of sediment attached pollutants is based on the Pollutant Partitioning Coefficients (PPCs) to associate pollutant concentrations to the two sediment fractions. The PPC concept assumes that pollutants in sediments do not accumulate under dry weather flows and that pollutants are only released when a sediment deposit is eroded. Any interactions between deposits and the flowing liquid are not considered.

The PPCs are used to relate sample results for real sediments to sediment fraction parameters for the model. The PPCs for each pollutant (BOD, COD and NH4) describe the distribution of pollutants in a volume of in situ sediment based on an estimate of the total pollution load *TP* for each sediment type.

The total pollutant load *TP* is expressed in units of mass of pollutants per litre of sediment with a specified bulk density. *TP* is partitioned into the following:

$$TP = DL + FL + CL \tag{5.1}$$

where:

DL	=	dissolved load associated with interstitial liquid,
FL	=	fine fraction load associated with particles < 0.5 mm,
CL	=	coarse fraction load associated with particles > 0.5 mm.

DL, FL and *CL* (the PPCs) are expressed as a percentage of *TP*.

When sediments are eroded the PPCs are used to add the load of pollutants released to the flow in the dissolved *DL* phase, the fine fractions *FL* and the coarse fractions *CL*. No further partitioning occurs under the subsequent transport, but the specified decay rates will be applied. If sediment deposition occurs, the bed sediment pollutant load (*TP*) and the PPCs as originally specified for the system are resumed.

Foul flow sediments are partitioned into dissolved load and a fine load already as a boundary condition. When deposition and erosion of possibly deposited foul flow sediments occur, the PPCs values for the pipe sediments are used (i.e. only the *DL* and the *FL*).

Use of the PPC concept requires that the BP module runs in parallel with the ST morphological model.

The mass at a specific site in the system is calculated from the initial sediment volumes at the bed and the PPC values specified according to:

$$
\begin{aligned}
Mass_{init,j} &= TP \cdot Bedsedimentvolume_{init,j} \\
DISSOLVED\ MASS_{init,j} &= Mass_{init,j} \cdot DL \\
FINE\ FRACTION\ MASS_{init,j} &= Mass_{init,j} \cdot FL \\
COARSE\ FRACTION\ MASS_{init,j} &= Mass_{init,j} \cdot CL
\end{aligned}
\tag{5.2}
$$

The transport of the sediment-attached pollutants is directly coupled to the sediment transport computations. Hence pollutant concentrations are evaluated from the amount of sediment in suspension.

When erosion and deposition occur, and fine sediment-attached pollutants are considered , the concentration in the water phase at specific location in the system is calculated from Equation (5.3):

$$
C_j = \frac{\dfrac{d\ Bedvolume}{dt} \cdot porosity \cdot FL + C_j \cdot V_j}{V_j}
\tag{5.3}
$$

where *Vj* is volume of the water body.

When pollutants attached to coarse sediments are calculated, Equation (5.4) is used:

$$
C_j = \frac{\dfrac{d\ Bedvolume}{dt} \cdot porosity \cdot CL + C_j \cdot V_j}{V_j}
\tag{5.4}
$$

When erosion occurs, the interstitial liquid which is eroded is added to the corresponding pollutant component in the water phase. This is solved by

including the eroded amount of dissolved pollutant (interstitial liquid) as a source term in the general Advection-Dispersion equation.

The *TP, DL, FL* and *CL* values are fixed in time and space. The amount of pollutant associated with the bed sediment is only dependent on the sediment transported in the system.

6 Build-up of Hydrogen Sulphide in Sewers

6.1 Introduction

Sewage has normally a high content of various organic and inorganic components, which are easily utilised by different types of microorganisms. The microbial transformation of organic compounds starts in the sewer network, where significant amounts of organic matter may be removed during transport (Ref. /8/). Hence, the sewer must be regarded as an integral part of the wastewater treatment system.

The dominating type of microbial activity in the sewer network will be determined by the composition and the concentration of the various components in the sewage, especially the concentration of electron acceptors (biological oxidants). The various available electron acceptors are utilised according to the fixed sequence; oxygen for aerobic respiration, nitrate for de-nitrification, organic compounds for fermentation, sulphate for sulphate reduction (sulphide production) and carbon dioxide for methanogenesis. Dissolved oxygen, ammonium, sulphate and organic compounds are natural components in sewage, while nitrate is usually not present in significant concentrations in domestic sewage (Ref. /8/).

Build-up sulphide in gravity sewers takes place mainly in large, slow flowing pipes with insufficient re-aeration at relatively high temperatures and - more often - in pressure mains, when the residence time of wastewater exceeds 1-2 hours. Industrial wastewater with high contents of organic matter and sulphur can contribute to the sulphide build-up.

In pressure mains with small diameters the production of sulphide mainly takes place in the biofilm on the pipe walls, whereas in sewers with large diameters anaerobic activity in the bulk liquid will also be of importance for the total generation of sulphide. The biological activity in the sediment in the sewer network can also be significant for the build-up of sulphide (Ref. /8/).

In Scandinavian climatic and typical structural conditions build-up of sulphide occurs in sewer pressure mains, reaching the concentrations of up to 10 mg S/l. Significantly higher concentrations are reported in other countries.

The sulphide production in sewers and modelling of this process is of interest due to the problems which may occur if the sulphide concentrations become high, including noxious odours with associated human health risk, corrosion of concrete and metal constructions and inhibition of sewer treatment processes Ref. /8/. Also, excessive content of sulphide may be toxic for fish in streams affected by overflow events /7/.

The following table can be used as a guideline for the impact of hydrogen sulphide presence in the air on human health.

Table 6.1   Assumable effects due to different sulphide concentrations (Ref. /10/)

Content of H_2S in the air [PPM]	Human reaction
< 0,13	Odourless
1	Minor odour
5	Distinct odour
10	Hygiene limit for one working day
10-50	Minor irritation of the eye
30	Strong obnoxious smell
50-100	Minor problems with eyesight and shortness of breath after just one hour
100-200	Problems with eyesight and coughing. Sense of smell disappears after 2-15 minutes and dizziness occurs after 14-30 minutes
500-1000	Rapid unconsciousness and death

The sulphide build-up model of MOUSE has been designed to analyze variations and build-up of sulphide in sewer networks during diurnal equilibrium. The testing of the model has given promising results in projecting the sulphide concentrations (Ref./7/).

6.2   The Model Concept

Investigations of sulphide formation in sewer systems have been carried out in the past and several predictive empirical models have been proposed. Several empirical models are listed in Table 6.2.

Table 6.2   Empirical equations for forecasting sulphide production rates. Unit for r_a is g/m^2/h[*]

Eq. no.		Reference
1	$r_a = 0.5 \cdot 10^{-3} u (C_{BOD_{Total}})^{0.8} \cdot (C_{SO_4^{2-}})^{0.4} \cdot 1.139^{(T-20)}$	Thistlethwayte, 1972
2	$r_a = 0.228 \cdot 10^{-3} C_{COD_{Total}} \cdot 1.07^{(T-20)}$	Boon & Lister, 1975

Table 6.2   Empirical equations for forecasting sulphide production rates. Unit for r_a is g/m²/h[*]

Eq. no.		Reference
3	$r_a = 1 \cdot 10^{-3} C_{BOD_{Total}} \cdot 1.07^{(T-20)}$	Pomeroy & Parkhurst, 1977
4	$r_a = k \cdot 10^{-3} (C_{COD_{Soluble}} - 50)^{0.5} \cdot 1.07^{(T-20)}$	Nielsen & Hvitved-Jacobsen, 1988

*) Can be expressed as g/m³/h by dividing with the hydraulic radius (V/A).

**) k = 1.5 for Danish domestic wastewater, 3 for wastewater with some contribution from food industry and 6 for easily degradable wastewater from food industry.

For models describing sulphide production in pressure mains the important parameters to quantify the sulphide production rate are the concentrations of sulphate, the concentrations of organic matter and the temperature. Organic matter is the key parameter because the sulphate concentration in wastewater is normally not the limiting factor for sulphide production (Ref. /11/). Typical concentrations of sulphate and sulphide in raw wastewater (Denmark) are approximately 20-100 mg/l and 0.1 mg/l, respectively (Ref. /12/).

Equations 2, 3 and 4 assume that the sulphate concentration is high and non-limiting, which usually is the case for concentrations above 4-5 mg SO4-S/l. In equations 2 and 3 the rate of H_2S production depends only on the concentration of total organic matter in the wastewater and the temperature, whereas Equation 1 also includes sulphate concentration and mean-flow velocity.

Equations 1 and 2 estimate maximum possible rates and they are a conservative result of measurements made in many pressure mains (Ref /14/). This also accounts for Equation 3, which is widely used in USA. This equation has been based on measurements from several sewer systems and it estimates the sulphide production rate under worst-case conditions (Ref./13/).

Equation 4 is useful for predicting variations in the sulphide production rate in a pressure main when it is known which type of wastewater is going to be modelled. It was proven suitable for estimating diurnal and seasonal variations in sulphide production in many Danish combined or separate pressure mains /8/.

Equation 4 has one major advantage for the application in MOUSE. Apart from the fact that dissolved COD is generally a better choice as a governing parameter in estimating sulphide build-up (bacteria use this fraction of COD predominantly), it is because dissolved COD is readily available component in MOUSE.

The sulphide modelling implementation in MOUSE includes all four empirical equations for sulphide build-up described above. It is possible to select any of the four equations depending on the situation that needs to be analysed and also depending on the available measured data. The latter is usually a decisive factor, since each of the four equations is dependent upon different measures of organic load.

Furthermore, Equation 1 depends on measurements of sulphate while the mean-flow velocity, which also enters the equation, is calculated in MOUSE. In Equations 1, 2 and 3 no calibration constants are applied, while Equation 4 includes a constant that represents the quality of the wastewater under analysis. In table 6-2 some guidelines are mentioned. Also, Ref. /11/ suggests that the hydrogen sulphide production rate is increased according to the following order (No. 1 has the largest rate while No. 3 has the lowest rate):

1. Wastewater from mainly food industries;

2. Wastewater from mixed municipal and industrial (food) sources;

3. Typical domestic wastewater (Denmark) with little or no content of industrial sewage.

The empirical models described above have limitations in describing the sulphide production. More fundamental (deterministic) models are required if the processes are to be described in more detail /11/.

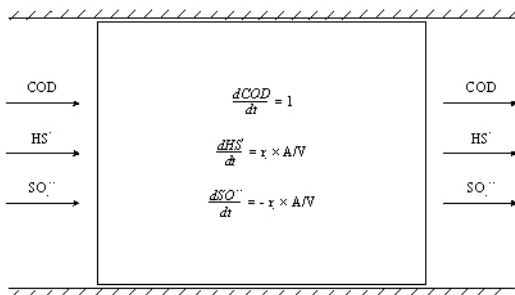Figure 6.1 illustrates the basic model concept implemented in MOUSE.

Figure 6.1   The basic model concept for the new sulphide module (HS-module)

When a pipe is full-running, it is possible to include a correction changing the production rate (r_a) to a negative value, i.e.:

$$r_a = -C_{HS} \cdot kst \tag{6.1}$$

where *kst* is a calibration constant.

6.3   Hydrogen Sulphide

The model described in the previous section computes sulphide build-up as the total sum of sulphide and hydrogen sulphide. To compute the concentration of the toxic gas hydrogen sulphide, the acidity (*pH*) is of great importance.

Hydrogen sulphide is in chemical equilibrium with sulphide according to the following equation:

$$H_2S \leftrightarrow HS^- + H^+ \leftrightarrow S^{2-} + 2H^+ \tag{6.2}$$

The chemical equilibrium between these three fractions is strongly dependent on *pH*. In wastewater, *pH* is normally between 6.6 and 7.2, and within this range the chemical equilibrium between H_2S and HS^- is very sensitive. A change of acidity within this interval by $\Delta pH = 0.2$ will create a change in the hydrogen sulphide concentration of about 30 % (Ref. /10/)

The implemented solution does not allow distinction between H_2S and HS^-.

Calculating the chemical equilibrium between sulphide (HS^-) and hydrogen sulphide (H_2S) (Ref. /12/), is presented in the following.

The chemical reaction:

$$H_2S \leftrightarrow HS^- + H^+ \tag{6.3}$$

Equilibrium is calculated as

$$\frac{[HS^-] \cdot [H^+]}{[H_2S]} = K \tag{6.4}$$

where:

$[HS^-]$	=	the concentration of sulphide,
$[H^+]$	=	the concentration of hydrogen,
$[H_2S]$	=	the concentration of hydrogen sulphide,
K	=	the equilibrium constant ($K = 9.12 \times 10^{-8}$ at 25°C).

Equilibrium is then dependent upon temperature and *pH*, as $pH = -log\,[H^+]$. The temperature dependency is described as:

$$\ln\left(\frac{K(T)}{K(T_0)}\right) = \frac{\Delta H}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right) \tag{6.5}$$

where:

R	=	the gas constant, R = 8.3144 J/mole/K
T	=	the actual temperature [K]
T_0	=	the temperature where K is known (25 °C)

$\Delta H = \Delta HS^- - \Delta H_2S = -16.3 + 38.6 = 22.3$ [KJ/mole]

6.4   The Z-Formula

An overall risk factor for the development of build-up of H_2S, Z, has been developed at DHI and has demonstrated good results in applications at a screening level. The equation implemented in MOUSE is:

$$Z = \frac{3 \cdot BOD_5 \cdot 1.07^{(T-20)}}{\sqrt{S \cdot Q}} \cdot \frac{P}{b} \qquad (6.6)$$

where:

$BOD5$	=	the biological oxygen demand after 5 days [g O_2/m^3],
T	=	the temperature in [°C],
S	=	the pipe slope [o/oo],
Q	=	the waste water discharge [l/sec],
B	=	the width of the water surface [m],
P	=	the wetted perimeter [m].

To avoid division by zero in the software, a minimum surface width is set to 0.01 meter.

Table 6.3   The risk producing H_2S in gravity sewers according to the Z-formula (b: surface width)

Lower limit	Parameter	Upper limit	Risk Assessment
0		5000	No risk
5000		10000	Possible H_2S production
10000	Z	25000	Large possibility of H_2S production
25000		∞	Guaranteed H_2S production

6.5   The WATS model

The WATS model is based on the integrated aerobic-anaerobic concept for microbial transformation investigated by Tanaka et al. (2000). The model is based on the model concept "Wastewater Aerobic/anaerobic Transformations in Sewers (WATS)" which was developed by Hvitved-Jacobsen et al. (1997) and Tanaka et al. (2000). The advantage of such model concept is the

capability to simulate aerobic as well as anaerobic processes including the transition between these two states seamlessly.

There are a lot of processes that influence the sulphide production in sewers. Since the investigation in the detail of sulphide production has started not so long ago, most of the processes are still unknown. The new model includes 7 main processes which are listed below. Such processes are already understood in certain level, while other processes such as the effect of nitrate still have to be more investigated.

- Aerobic growth in bulk water and biofilm: the growth of bacteria in sewers that utilize the substrate in the wastewater.

- Maintenance energy requirement: the minimum energy for bacteria metabolism which is needed to survive.

- Aerobic/anaerobic hydrolysis: the hydrolysis of hydrolysable substrate to readily biodegradable substrate.

- Fermentation: the fermentation of fermentable biodegradable substrate to fermentation products (Volatile Fatty Acid, VFA).

- Sulphide formation: the formation of hydrogen sulphide in biofilm.

- Sulphide release to gaseous phase: the dissolved hydrogen sulphide gas escaping from the bulk water.

- Reaeration: the oxygen transfer between air above wastewater in the gravity sewer.

One of the differences between the new and the empirical models is data input. For empirical models, COD or BOD is input directly as organic source while the new model uses the fraction of readily degradable substrate. Theoretically, the usage of COD fraction is more accurate and the OUR experiment is then needed to determine the parameters. However, for some models where OUR experiment is absent, the limitation of data availability causes inapplicability of the model. So, to avoid this problem, the new model is developed with the ability to put the average default values as the proportions for each fraction of COD in ADP file.

Based on information from Tanaka 2002 Figure 6.2 shows the concept of the processes in the WATS model.
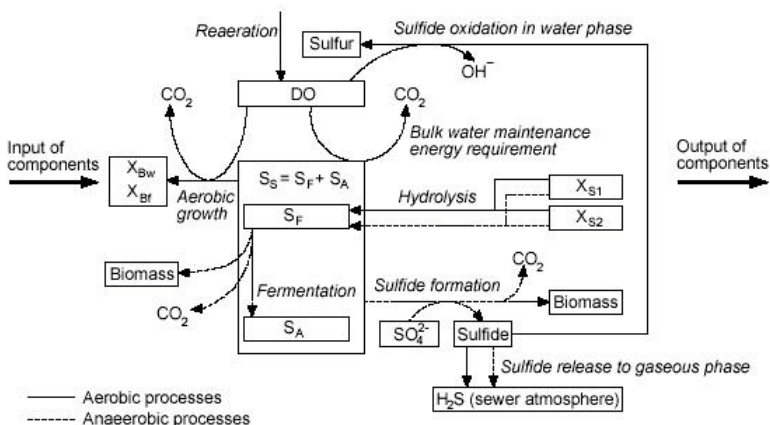
Figure 6.2　Integrated aerobic-anaerobic concept for microbial transformations of organic carbon and sulfur in sewers (Tanaka et al., 2000)

The equation matrix applied in the WATS model can be seen below.

Table 6.4　Model matrix investigated by Tanaka et al., 2000

Process	1 S_F	2 S_A	3 XB_w	4.1 X_{S1}	4.2 X_{S2}	5 -S_O	6 S_{H2S}	Process rate
Aerobic growth in bulk water	$-1/Y_{Hw}$	1				$(1-Y_{Hw})/Y_{Hw}$		Equation (a)
Aerobic growth in biofilm	$-1/Y_{Hf}$	1				$(1-Y_{Hf})/Y_{Hf}$		Equation (b)
Mainte-nance energy require-ment		-1	-1*					Equation (c)
Aerobic hydrolysis, fast (X_{S1})	1			-1				Equation (d), # = 1
Aerobic hydrolysis, slow (X_{S2})	1				-1			Equation (d), # = 2
Anarobic hydrolysis, fast (X_{S1})	1			-1				Equation (e), # = 1

Table 6.4   Model matrix investigated by Tanaka et al., 2000

Process	1 S_F	2 S_A	3 XB_w	4.1 X_{S1}	4.2 X_{S2}	5 $-S_O$	6 S_{H2S}	Process rate
Anarobic hydrolysis, slow (XS2)	1				-1			Equation (e), # = 2
Fermentation in bulk water & biofilm	-1	1						Equation (f)
Sulfide formation in biofilm		-2					1	Equation (g)
Sulfide oxidation						0.5	-1	Equation (h)
Sulfide release to gaseous phase							-1	Equation (i)
Rearation						-1		Equation (j)

* If S_F+S_A is not sufficiently available to support maintenance energy requirement.

Aerobic growth in bulk water and biofilm: the growth of bacteria in sewers that utilize the substrate in the wastewater.

Maintenance energy requirement: the minimum energy for bacteria metabolism which is needed to survive.

Aerobic/anaerobic hydrolysis: the hydrolysis of hydrolysable substrate to readily biodegradable substrate.

Fermentation: the fermentation of fermentable biodegradable substrate to fermentation products (Volatile Fatty Acid, VFA).

Sulfide formation: the formation of hydrogen sulfide in biofilm.

Sulfide oxidation: the conversion from sulfide to sulfate.

Sulfide release to gaseous phase: the dissolved hydrogen sulfide gas escaping from the bulk water.

Reaeration: the oxygen transfer between air above wastewater in the gravity sewer.

$$\mu_H \cdot \frac{(S_F + S_A)}{K_{Sw} + (S_F + S_A)} \cdot \frac{S_O}{K_O + S_O} \cdot X_{Bw} \alpha_w^{(T-20)} \tag{6.6a}$$

$$\frac{Y_{Hf}}{(1 - Y_{Hf})} \cdot \frac{(S_F + S_A)}{K_{Sf} + (S_F + S_A)} \cdot \frac{A_{W-P}}{V} \cdot k_{1/2} S_O^{0.5} \alpha_f^{(T-20)} \tag{6.6b}$$

$$q_m \cdot \frac{S_O}{K_O + S_O} \cdot X_{Bw} \alpha_w^{(T-20)} \tag{6.6c}$$

$$k_{h\#} \cdot \frac{(X_{S\#}/X_{Bw})}{K_{X\#} + (X_{S\#}/X_{Bw})} \cdot \frac{S_O}{K_O + S_O} \cdot \left(X_{Bw} + \varepsilon_A X_{Bf} \frac{A_{W-P}}{V}\right) \alpha_w^{(T-20)} \tag{6.6d}$$

$$\eta_{fe} \cdot k_{h\#} \cdot \frac{(X_{S\#}/X_{Bw})}{K_{X\#} + (X_{S\#}/X_{Bw})} \cdot \frac{K_O}{K_O + S_O} \cdot \left(X_{Bw} + \varepsilon_{An} X_{Bf} \frac{A_{W-P}}{V}\right) \alpha_w^{(T-20)} \tag{6.6e}$$

$$q_{fe} \cdot \frac{S_F}{K_{fe} + S_F} \cdot \frac{K_O}{K_O + S_O} \cdot \left(X_{Bw} + \varepsilon_{An} X_{Bf} \frac{A_{W-P}}{V}\right) \alpha_w^{(T-20)} \tag{6.6f}$$

$$k_{nS} \cdot S_F^n \cdot \frac{K_{O(S)}}{K_{O(S)} + S_F} \cdot \frac{A_{W-P}}{V} \cdot \alpha_f^{(T-20)} \tag{6.6g}$$

$$P_s \cdot \frac{i \cdot S_{H2S}}{K_{H2S} + i \cdot S_{H2S}} \cdot \frac{S_O}{K_O + S_O} \cdot \alpha_w^{(T-20)} \tag{6.6h}$$

$$0.69(1 + 0.17 Fr^2)(s \cdot u)^{3/8}(j \cdot i \cdot S_{H2S}) \cdot d_m^{-1} \cdot \alpha^{(T-20)} \tag{6.6i}$$

$$K_{La}(S_{OS} - S_O) \tag{6.6j}$$

Nomenclature for the WATS model

A_{W-P} Wastewater-Pipe surface area [m²]

d_m Hydraulic mean depth [m]

Fr Froude number

i Proportion of dissolved sulphide to total sulphide

j Proportion of dissolved sulphide present as H2S

$k_{n\#}$Hydrolysis rate constant, fraction # [d-1]

k_{nS}n order rate constant for sulphide formation [gn/mn·h]

KfeSaturation constant for fermentation [g COD/m^3]

K_{H2S}Saturation constant for sulphide oxidation [g S/m^3]

K_{La}Oxygen transfer coefficient [h-1]

K_OSaturation rate constant for dissolved oxygen [g O2/m^3]

$K_{O(S)}$Saturation rate constant for dissolved oxygen inhibition [g O2/m^3]

K_{Sf}Saturation constant for Ss in the biofilm [g COD/m^3]

K_{Sw}Saturation constant for Ss in the water phase [g COD/m^3]

$K_{X\#}$Saturation constant for hydrolysis, fraction # [g COD/g COD]

$k_{1/2}$Half order rate constant for aerobic growth in the biofilm [g O20.5/m0.5·d]

nReaction order

p_sRate constant for sulphide oxidation in the water phase [g S/m3·h]

q_{fe}Maximum rate for fermentation [d-1]

q_mMaintenance energy requirement rate constant [d-1]

sSlope of gravity sewer [m/m]

S_AFermentation products [g COD/m^3]

S_FFermentable, readily biodegradable substrate [g COD/m^3]

S_{H2S}Total sulfide concentration [g S/m^3]

S_ODissolved oxygen [g O2/m^3]

S_{OS}Dissolved oxygen saturation constant [g O2/m^3]

TTemperature [ºC]

uMean flow velocity [m/s]

VWastewater volume [m^3]

X_{Bf}Heterotrophic active biomass in the biofilm [g COD/m^2]

X_{Bw}Heterotrophic active biomass in the water phase [g COD/m^3]

$X_{S\#}$ Hydrolysable substrate, fraction # [g COD/m³]

Y_{Hf} Biofilm yield constant for heterotrophic biomass [g COD/g COD]

αf Temperature coefficient in the biofilm = 1.03

αT Temperature coefficient for re-aeration = 1.024

α_w Temperature coefficient in the water phase = 1.07

ε_A Efficiency constant for the biofilm biomass under aerobic conditions

ε_{An} Efficiency constant for the biofilm biomass under anaerobic conditions

ηfe Anaerobic hydrolysis reduction factor

µ Maximum specific growth rate for heterotrophic biomass [d-1]

Fraction of hydrolysable substrate, # = 1: fast hydrolysable, # = 2: slowly hydrolysable

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