Improvement of Energy Efficiency for Wastewater Treatment

Report Contributors: Mark Burke¹, Michael Chapwanya^{2,3}, Kevin Doherty⁴, Ian Hewitt ⁵, Andrei Korobeinikov², Martin Meere⁶, Stephen McCarty ⁷, Mick O'Brien², Vo Thi Ngoc Tuoi⁶ and Henry Winstanley^{2,5}

Industry Representatives: Toshko Zhelev⁸ and Jaime Rojas⁸

¹Department of Mathematics and Statistics, University of Limerick, Ireland

⁴National University of Ireland Galway, Ireland

 $^{^2 \}rm MACSI,$ Department of Mathematics and Statistics, University of Limerick, Ireland $^3 \rm Report$ coordinator, m.chapwanya@ul.ie

⁵OCIAM, Mathematical Institute, University of Oxford, United Kingdom

⁶Department of Applied Mathematics, National University of Ireland Galway, Ireland ⁷University College Cork, Ireland

⁸Department of Chemical and Environmental Science, University of Limerick, Ireland

Abstract

Wastewater treatment requires the elimination of pathogens and reduction of organic matter in the treated sludge to acceptable levels. One process used to achieve this is Autothermal Thermophylic Aerobic Digestion (ATAD), which relies on promoting non-pathogenic thermophilic bacteria to digest organic matter and kill pathogens through metabolic heat generation. This process requires continuous aeration that may be energy consuming, and the final aim of the study is to identify how the process design can minimize the energy input per mass of treated sludge. Appropriate modeling of the reactor process is an essential ingredient, so we explore properties of an existing model and propose a simplified alternative model.



(a) A single-reactor design. An example of this design is found in Spain.



(b) A two-reactor design. Semi continuous or continuous treatment requires multiple reactors to achieve pasteurization. An example of this design is found in Killarney, Ireland.

1 Introduction

1.1 Background

Wastewater treatment employs a variety of processes to reduce the environmental and health impacts of effluent. Treatment is an environmental necessity but is itself very energy-intensive, and this energy use is one of the principal costs and environmental impacts of the treatment. Wastewater impurities include a wide range of inorganic and organic chemical species and microorganisms. A filtered, concentrated 'sludge' is produced at initial stages of treament. A key subsequent stage is to eliminate potential pathogenic organisms and reduce the organic chemical content which might act as a substrate for further microbial growth. One process that is used to achieve these treatment goals is autothermal thermophilic aerobic digestion (ATAD).

ATAD makes use of bacterial growth within the sludge both to reduce organic chemical content and to kill pathogenic bacteria. Aeration of the sludge promotes the growth of aerobic bacteria which feed on and reduce the organic substrates available in the sludge. This metabolic activity generates heat and raises the temperature of the sludge. Thermophilic bacteria in the sludge thrive at high temperatures (Fig. 1). Most pathogens, meanwhile, are mesophiles: their total metabolic activity reduces rapidly at temperatures above 40 - 45 °C, and they are eventually killed by sufficiently long exposure (Fig. 2). Aerobic thermophiles proliferate and dominate in the hot sludge, and ATAD uses their metabolic activity and heat generation to achieve the treatment goals of pasteurization and reduction of organics.



Figure 1: Temperature dependence of the thermophilic growth and decay rate (adapted from [6]).

The time and cost implications of running full-scale experiments for different plant arrangements and operating conditions render such an approach infeasible for process design and operational management. Laboratory scale experiments have provided understanding (to varying degree) of many of the microbiological and chemical processes involved. By encapsulating much of this



Figure 2: Temperature dependence of the mesophilic growth and decay rate (adapted from [6]).

understanding in mathematical models, engineers have provided tools which allow computer simulations to inform the design process. The 'Activated Sludge Model 1' (ASM1) [5] and subsequent variants [3, 4] have achieved a broad level of acceptance in the wastewater treatment world. Based on the dominance of the ASM1 model (and family) in the field, its extension to the ATAD process as set out by [6, 2] appears to have created a *de facto* standard for modeling this process, despite drawbacks summarized below. We identify this existing model with the label ASM1.

1.2 Objective

The intended purpose of the Study Group problem was to use a model of the ATAD treatment process to provide insights into the optimization of both plant design and operating conditions in order to reduce the energy consumed per mass of treated sludge while achieving the required treatment goals.

Approaching the problem as a multidimensional constrained optimization based on the ASM1 model, the problem presenters had identified some generic indications for performance improvements, but encountered numerical difficulties due to the high dimensionality and sensitivity to parameters inherent in the ASM1 model. Their next intention was to identify rational means of reducing the dimensionality of the optimization.

1.3 Report Overview

This report addresses the problem in the following way:

• Section 2 provides a more detailed overview of the problem and the considerations raised

during the Study Group.

- In Section 3 we discuss the ASM1 model, perform a nondimensionalization based on typical parameter values (adapted from [2] and [6]), and identify certain regimes within the timecourse of a single typical batch reaction for which asymptotic approximations may be appropriate.
- In Section 4 we present a simplified 'ESGI70' model proposed by the Study Group with the intention of being the minimal model required to describe the observed process. The model comprises a system of ODEs with four dependent variables.
- In Section 5 we compare our simulations to experiments and present a sensitivity analysis of the ESGI70 model.
- In Section 6 we present an optimal strategy for pasteurization.

2 Problem Overview

2.1 Treatment Goals

Legal requirements for sludge treatment in Ireland and USA set minimum standards for the pasteurization and stabilization of the treated outflow sludge ([8]). Stabilization refers to the reduction of volatile solids concentration between sludge intake X_{vs}^{feed} and outflow X_{vs}^{out} , and the required minimum reduction is set at 38%:

$$\frac{X_{\rm vs}^{\rm feed} - X_{\rm vs}^{\rm out}}{X_{\rm vs}^{\rm feed}} \geq 0.38.$$
(2.1)

Pasteurization is achieved by the sludge being subjected to high temperature for a prolonged period of time. Rather than requiring direct microbiological testing of the outflow, the legal requirement for pasteurization specifies a minimum value of 1.0 for a derived 'lethality' statistic which is an empirically-based function of sludge temperature and time elapsed in the ATAD reaction process:

$$L(T,t) = \int_{t_0}^{t} \frac{1}{a} 10^{bT(t)} dt \ge 1, \qquad (2.2)$$

where temperature T is measured in Celsius, elapsed time t in days, and $a = 5.007 \times 10^7$ and $b = 0.14 \,^{\circ}C^{-1}$ are defined parameter values. Lethality L is only calculated in continuous time intervals in which temperature $T > 50 \,^{\circ}C$, and it is equal to zero when $T \le 50 \,^{\circ}C$.



Figure 3: Schematic representation of a reactor. The ATAD process must have a feed control mechanism which ensures that the organic feed is above a certain minimum concentration for adequate heat production. The solids must also be below a maximum concentration to allow adequate mixing. See for example [8].

2.2 Treatment Plant and Process

ATAD is operated as a batch or semi-batch process. A large reactor containing sludge receives an additional volume of untreated sludge at the start of a batch via a feed inlet (see schematic in Fig. 3). During the batch reaction air is pumped continuously into the reactor and provides both the oxygenation required for aerobic bacterial growth and the physical mixing of the sludge in the whole reactor. Digestion of organic substrates proceeds hand in hand with bacterial growth, predominantly of thermophiles due to the elevated temperature. At the end of the batch reaction time, a volume of treated outflow sludge is removed and is immediately replaced by the next batch of intake sludge. Thus the outflow sludge has the same composition as the mixed sludge in the reactor at the end of the batch reaction time t_{batch} . Batch outflow and inflow cannot be open at the same time since untreated inflow sludge might be drawn off with and taint the outflow sludge. The time between successive batch intakes is typically fixed at 24 hours for staffing reasons. In order to achieve the desired treatment outcomes, treatment plant designs may include a single ATAD reactor stage, or two reactors in series with outflow from the first reactor being inflow into the second. In some cases, the treatment plant consist of an ATAD reactor and an anaerobic mesophilic digester in series (cf. [8]). The method of operation and the number of reactors used depends on the fluctuation of hydraulic loading and on the quantity of sludge requiring treatment.

2.3 Optimization

As indicated in Section 1.2, the primary objective is to optimize the plant design and operating conditions so that the minimum energy consumed per mass of treated sludge. The plant's energy consumption is dominated by the submerged aeration pumps' energy requirements. For a sludge aeration rate A (air volumes per reactor sludge volume per day), reactor volume V, and batch inflow (and outflow) volume V_{in} , the optimization corresponds to finding the set of controls U which yield

$$\min_{\mathbf{U}} \frac{V}{V_{\text{in}}} \int \mathbf{A}(\mathbf{t}) d\mathbf{t}, \tag{2.3}$$

subject to the treatment requirement constraints Eqs. (2.1),(2.2). The full range of optimization controls U comprises both plant design issues and operating conditions. Design choices include reactor volume and the use of single or series reactors. Other non-standard possibilities can also be assessed such as parallel heat exchangers to pre-warm the sludge inflow from sludge outflow, reactor, or exhaust air heat sources. Controls on operating conditions in the reactor are limited to the aeration rate and batch reaction time t_{batch} , and controls on the batch inflow volume, temperature and substrate concentration. For staffing reasons, current standard operating conditions generally use a 24-hour batch cycle and maintain a constant aeration rate A during the whole process. The inflow volume can be expressed as a reactor batch exchange fraction $Q = V_{in}/V \in (0, 1]$ and is typically in the range 0.1 - 0.2. The inflow is usually at ambient temperature and existing plants are not set up for inflow heating either directly or by heat exchangers. The substrate concentration of inflow sludge can be increased by addition of a bulking organic component at minimal expense.

2.4 Study Group Approach

As with many biological systems, there is considerable uncertainty in inferring both the functional description of processes and the accuracy of parameterizations when applying laboratoryderived models to the real system. The current models in the wastewater literature are motivated by microbiological and engineering interest and have been devised to incorporate as much as possible of the apparent understanding of underlying processes. As a result they tend to include a relatively large number of variables, processes, and parameters.

This stands in contrast to the paucity of data accessible from ATAD plants in operation: aeration rate and sludge temperature are easily monitored, but data on sludge composition at inlet and outlet and during the course of the batch reaction is typically limited to the total dry weight of solids and the chemical oxygen demand of the 'volatile solids' (by controlled chemical oxidation of the sludge). Volatile solids include the biomass of bacteria in the sludge together with organic growth substrates and metabolically inert organic compounds, so no distinction is made between these components in the measured data.

In addition to the known model being over-parameterized, commonly-used values of several

parameters are inferred from curve-fitting predicated on the model itself. In such an exercise, the discrepancy between the large numbers of variables and parameters in the model and their poor representation in the available data clearly motivates the use of a simplified model of the process.

The key focus of the Study Group was modeling the core process of a single reactor system during a batch reaction. Such a model is trivially set up to run successive batches and can easily be extended later to a multi-reactor system and other design variants. Two approaches were followed: one being to investigate the existing ASM1 model for mathematical simplifications (Section 3), the other being to construct a new model using a plausible minimal set of interactions to see if it can reproduce the observed behavior (Section 4).

The optimization of the process based on such a model was not fully addressed in the Study Group, though some sensitivity analysis and initial investigations into its optimization were tackled. The focus on the core process model and the relative lack of suitably realistic estimates for many of the plant-specific parameters suggested greater priority be placed on single reactor operating conditions as optimization controls. Thus the initial focus was on a single reactor system of fixed design, with plant design optimization left as a task for future work.

2.5 Basic Modeling Assumptions

Some simplifying assumptions permit us to reduce the complexity of the model while at the same time retaining the essential aspects of the processes:

- There is complete mixing inside the reactor(s).
- All the biological activity takes place only in the reactors.
- The batch outflow and inflow stages are of sufficiently short duration that biological activity during them is negligible.
- Aeration is sufficient that anaerobic metabolic activity is negligible.

3 The Existing ASM1 Model

The ASM1 model incorporates all the processes identified by microbiologists as being relevant to modeling the ATAD process. A transfer diagram of the ASM1 model is shown in Fig. 4 with the solid curve cycle showing the processes included in the original ASM1 model (prior to the ATAD extension). Here $X_{\rm BH}$ denotes the concentration of active mesophilic biomass, $S_{\rm o}$ is the concentration of oxygen and $X_{\rm P}$ is the concentration of inert organic matter. Organic substrate is separated into readily biodegradable substrate $S_{\rm s}$ and slowly degradable substrate $X_{\rm s}$. Untreated sludge in the batch inflow contains a certain concentration of both these substrates. The slow substrate X_s consists of organic macromolecules which can be hydrolyzed to produce the fast substrate S_s . Microbial decay adds to the pool of X_s : cell lysis on death releases the cell's constituents into the extracellular space, a fraction f_P of which is inert matter and $(1 - f_P)$ is hydrolyzable macromolecular substrate. Fast substrate S_s and oxygen S_o are consumed in growth of the bacteria. All the metabolic process rates are assumed to depend nonlinearly on substrate and oxygen concentrations through dual Michaelis–Menten kinetics terms.

The ATAD-specific modifications to the ASM1 model are (broken curve cycle in Fig. 4) via the introduction of a new component: thermophilic biomass, in active X_{BHT} and inactive X_{SP} forms. While mesophiles are relevant to batch reactions starting from cold, typical ATAD plants are operated with batches following in rapid succession precisely in order to maintain the temperature of the reactor. Under these conditions, the mesophiles respire but the temperatures are beyond their optimum level and so they decay very fast and thus do not make noticeable contribution to the process, see Fig. 2.



Figure 4: Transfer diagram of the processes in the ASM1 model (solid lines) and the proposed extended model (broken lines). In Section 3.1 we present the mathematical representation of the extended model. (adapted from [7])

3.1 The ASM1 Model at Thermophilic Temperatures

The ASM1 model at thermophilic temperatures tracks the evolution in time of eight quantities in the reactor, these being: $S_s(t)$ the readily biodegradable substrate, $X_s(t)$ the slowly biodegradable substrate, $X_{\rm SP}(t)$ the inactivate thermophilic biomass, $X_{\rm BH}(t)$ the active mesophilic biomass, $X_{\rm BHT}(t)$ the active thermophilic biomass, $X_{\rm P}(t)$ inert organic matter from decay, $S_o(t)$ the dissolved oxygen, and T(t) the temperature. For simplicity, we disregard the temperature dependence here, and so do not display an equation for the temperature. We take fixed values for the model parameters and choose these values for reactor operation at 50°C. We also neglect the effect of thermophilic activation, on the basis that it occurs rapidly at the start of the batch reaction, and so do not consider inactive biomass $X_{SP}(t)$ in the model. Under these assumptions, the governing equations from [6] are

$$\begin{split} \frac{dS_{s}}{dt} &= -\frac{1}{Y_{H}} \mu_{H} \frac{S_{s}}{K_{s} + S_{s}} \frac{S_{o}}{K_{o} + S_{o}} X_{BH} - \frac{1}{Y_{HT}} \mu_{HT} \frac{S_{s}}{K_{ST} + S_{s}} \frac{S_{o}}{K_{OT} + S_{o}} X_{BHT} \\ &+ k_{H} \frac{X_{s}}{K_{x} X_{BH} + X_{s}} \frac{S_{o}}{K_{o} + S_{o}} X_{BH} + k_{HT} \frac{X_{s}}{K_{xT} X_{BHT} + X_{s}} \frac{S_{o}}{K_{OT} + S_{o}} X_{BHT}, \\ \frac{dX_{s}}{dt} &= b_{H} (1 - f_{P}) X_{BH} + b_{HT} (1 - f_{PT}) X_{BHT} - k_{H} \frac{X_{s}}{K_{x} X_{BH} + X_{s}} \frac{S_{o}}{K_{o} + S_{o}} X_{BH} \\ &- k_{HT} \frac{X_{s}}{K_{xT} X_{BHT} + X_{s}} \frac{S_{o}}{K_{OT} + S_{o}} X_{BHT}, \\ \frac{dX_{BH}}{dt} &= \mu_{H} \frac{S_{s}}{K_{s} + S_{s}} \frac{S_{o}}{K_{O} + S_{o}} X_{BH} - b_{H} X_{BH}, \\ \frac{dX_{BHT}}{dt} &= \mu_{HT} \frac{S_{s}}{K_{sT} + S_{s}} \frac{S_{o}}{K_{O} + S_{o}} X_{BHT} - b_{HT} X_{BHT}, \\ \frac{dS_{o}}{dt} &= -\frac{(1 - Y_{H})}{Y_{H}} \mu_{H} \frac{S_{s}}{K_{s} + S_{s}} \frac{S_{o}}{K_{O} + S_{o}} X_{BH} - \frac{(1 - Y_{HT})}{Y_{HT}} \mu_{HT} \frac{S_{s}}{K_{ST} + S_{s}} \frac{S_{o}}{K_{OT} + S_{o}} X_{BHT} \\ &+ k_{La} \left(\bar{S_{o}} - S_{o}\right), \\ \frac{dX_{P}}{dt} &= f_{P} k_{H} \frac{X_{s}}{K_{x} X_{BH} + X_{s}} \frac{S_{o}}{K_{O} + S_{o}} X_{BH} + f_{PT} k_{HT} \frac{X_{s}}{K_{xT} X_{BHT} + X_{s}} \frac{S_{o}}{K_{OT} + S_{o}} X_{BHT}. \end{split}$$

The parameters appearing in the model are explained in Table 5. We see that the first five of these equations can be solved independently of the sixth, and so we do not display the equation for the inert organic matter $X_{\rm P}$ again.

We model the operation of a single tank system for one batch, and so solve $(3.1)_1 - (3.1)_5$ subject to initial conditions

$$S_{\rm s} = S_{\rm s}^{\rm o}, X_{\rm s} = X_{\rm s}^{\rm o}, X_{\rm BH} = X_{\rm BH}^{\rm o}, X_{\rm BHT} = X_{\rm BHT}^{\rm o}, S_{\rm o} = S_{\rm o}^{\rm o} \text{ at } t = 0.$$
 (3.2)

For the illustrative numerical results used in the current analysis, we take

$$S_{\rm s}^{\rm o} = 5 \text{ gl}^{-1}, \ X_{\rm s}^{\rm o} = 15 \text{ gl}^{-1}, \ X_{\rm BH}^{\rm o} = 1 \text{ gl}^{-1}, \ X_{\rm BHT}^{\rm o} = 1 \text{ gl}^{-1}, \ S_{\rm o}^{\rm o} = 10^{-3} \text{ gl}^{-1}.$$

We scale the system of ordinary differential equations by choosing

$$t \sim t_{\rm batch}, \ S_{\rm S} \sim S_{\rm S}^o, \ X_{\rm S} \sim X_{\rm S}^o, \ X_{\rm BH} \sim X_{\rm BH}^o, \ X_{\rm BHT} \sim X_{\rm BHT}^o, \ S_{\rm O} \sim S_{\rm O}^o,$$

where $t_{\text{batch}} = 1 \text{ d}$ (one day). With this choice of scaling, the dimensionless form for $(3.1)_{1}$ -

 $(3.1)_5$, (3.2) is given by,

$$\begin{aligned} \frac{dS_{s}}{dt} &= -\delta_{1} \frac{S_{s}}{\delta_{2} + S_{s}} \frac{S_{o}}{\delta_{3} + S_{o}} X_{BH} - \delta_{4} \frac{S_{s}}{\delta_{5} + S_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{BHT} \\ &+ \delta_{7} \frac{X_{s}}{\delta_{8} X_{BH} + X_{s}} \frac{S_{o}}{\delta_{3} + S_{o}} X_{BH} + \delta_{9} \frac{X_{s}}{\delta_{10} X_{BHT} + X_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{BHT}, \\ \frac{dX_{s}}{dt} &= \delta_{11} X_{BH} + \delta_{12} X_{BHT} - \delta_{13} \frac{X_{s}}{\delta_{8} X_{BH} + X_{s}} \frac{S_{o}}{\delta_{3} + S_{o}} X_{BH} - \delta_{14} \frac{X_{s}}{\delta_{10} X_{BHT} + X_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{BHT}, \\ \frac{dX_{BH}}{dt} &= \delta_{15} \frac{S_{s}}{\delta_{2} + S_{s}} \frac{S_{o}}{\delta_{3} + S_{o}} X_{BH} - \delta_{16} X_{BH}, \\ \frac{dX_{BHT}}{dt} &= \delta_{17} \frac{S_{s}}{\delta_{5} + S_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{BHT} - \delta_{18} X_{BHT}, \\ \frac{dS_{o}}{dt} &= -\delta_{19} \frac{S_{s}}{\delta_{2} + S_{s}} \frac{S_{o}}{\delta_{3} + S_{o}} X_{BH} - \delta_{20} \frac{S_{s}}{\delta_{5} + S_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{BHT} + \delta_{21} (\delta_{22} - S_{o}), \end{aligned}$$

$$(3.3)$$

subject to initial conditions

$$S_{\rm\scriptscriptstyle S} = 1, \, X_{\rm\scriptscriptstyle S} = 1, \, X_{\rm\scriptscriptstyle BH} = 1, \, X_{\rm\scriptscriptstyle BHT} = 1, \, S_{\rm\scriptscriptstyle O} = 1 \ \, {\rm at} \ \, t = 0, \label{eq:S_s}$$

where the definition of, and values for, the non-dimensional parameters δ_i $(1 \le i \le 22)$ are given in Table 5.

In Figs. 5 and 6, we show the solution to the system of equations (3.3) for the parameter values listed in Table 5. It is noteworthy from the parameter values chosen, the readily degradable material is depleted over a period of approximately one half of a day, but that the slowly degradable material persists for approximately five days. We should note, however, that that some of the parameter values used are uncertain, and that they can depend on temperature and time, as well as other factors, such as the character of the inflow sludge and the reactor system. Since we have assumed the parameter values to be fixed, the limitations of such an approach are clear. However, our goal in this section is to gain some insight into aspects of the ASM1 model, rather than attempting to model a particular reactor system in detail.

3.2 A Subcase: Asymptotic Analysis of the ASM1 Model

As mentioned above, under normal ATAD operating conditions a relatively high temperature is maintained in the reactor. Commonly, the temperature after adding a new inflow batch and mixing remains higher than the mesophilic temperature range, and hence their metabolic activity is negligible. Therefore we neglect mesophiles in the model and set $X_{BH} = 0$; equations



Figure 5: Plot of the solution to system of equations (3.3) over one day and for the parameter values displayed in Table 5.



Figure 6: The same solution as in Figure 5, plotted over one week. Over this time, the slowly biodegradable substrate is removed, and the dissolved oxygen achieves its saturation value.

\mathbf{S} ymbol	Description	Value	Units			
Physical parameters						
K _s	mesophilic half saturation constant for S_s	0.02	g/l			
Ko	mesophilic half saturation constant for $S_{\rm o}$	$2 imes 10^{-4}$	g/l			
$K_{\rm ST}$	thermophilic half saturation constant for $S_{\rm s}$	0.03	g/l			
$K_{\rm OT}$	thermophilic half saturation constant for $S_{\rm o}$	$2 imes 10^{-4}$	g/l			
$\bar{s_o}$	oxygen saturation concentration	$5 imes10^{-3}$	g/l			
$\mu_{ m H}$	maximum growth rate of $X_{\rm BH}$	16.8	1/d			
$\mu_{\rm HT}$	maximum growth rate of X_{BHT}	24.3	1/d			
$b_{\rm H}$	decay rate of mesophiles	43	1/d			
$b_{\rm HT}$	decay rate of thermophiles	5.2	1/d			
$k_{\rm H}$	maximum mesophilic hydrolysis rate	10	1/d			
$k_{\rm HT}$	maximum thermophilic hydrolysis rate	9.2	1/d			
k_{La}	oxygen mass transfer coefficient	1000	1/d			
$Y_{\rm H}$	mesophilic yield	0.6	—			
$Y_{\rm HT}$	thermophilic yield	0.6	_			
f _P	inert fraction of mesophilic biomass	0.3	_			
$f_{\rm PT}$	inert fraction of thermophilic biomass	0.3	_			
K _x	half saturation constant for mesophilic hydrolysis	0.03	_			
$K_{\rm XT}$	half saturation constant for thermophilic hydrolysis	0.03	—			

Table 4: The set of parameters for the ASM1 model, physical parameters. Experiments have shown that these parameters can depend, among other things, on temperature and time (see Figs. 1 and 2).

Table 5: The set of parameters for the ASM1 model, dimensionless parameters. Experiments have shown that these parameters can depend, among other things, on temperature and time (see Figs. 1 and 2). Here we assume these parameters to be constant (i.e., temperature independent).

\mathbf{S} ymbol	Description	Value	Units	
	Dimensionless parameter	ers		
δ_1	$\mu_{ m H} { m t}_{ m batch} { m X}^{ m o}_{ m BH}/({ m Y}_{ m HT} { m S}^{ m o}_{ m S})$	5.60	-	
δ_2	K_s/S_s^o	4×10^{-3}	_	
δ_3	K_o/S_o^o	0.2	—	
δ_4	$\mu_{\rm HT} t_{\rm batch} X^o_{\rm BHT} / (Y_{\rm HT} S^o_{\rm S})$	8.10	—	
δ_5	$K_{\rm ST}/S^{\rm o}_{\rm S}$	6×10^{-3}	—	
δ_6	K_{OT}/S_{O}^{o}	0.2	—	
δ_7	$k_{\rm H} t_{\rm batch} X_{\rm BH}^* / S_{\rm S}^*$	2.0	—	
δ_8	${\sf K}_{ m x}{\sf X}^{ m o}_{ m BH}/{\sf X}^{ m o}_{ m s}$	2×10^{-3}	—	
δ9	$\left(\mathrm{k_{\scriptscriptstyle HT}}\mathrm{t_{\scriptscriptstyle batch}} ight)\left(\mathrm{X^*_{\scriptscriptstyle BHT}}/\mathrm{S^o_{\scriptscriptstyle S}} ight)$	1.84	—	
δ_{10}	$K_{\rm XT}X^{o}_{\rm BHT}/X^{o}_{\rm S}$	2×10^{-3}	—	
δ_{11}	$(1-f_{\scriptscriptstyle \mathrm{P}})b_{\scriptscriptstyle \mathrm{H}}t_{\scriptscriptstyle \mathrm{batch}}X^o_{\scriptscriptstyle \mathrm{BH}}/X^o_{\scriptscriptstyle \mathrm{S}}$	2.01	—	
δ_{12}	$(1-f_{\scriptscriptstyle \mathrm{PT}})b_{\scriptscriptstyle \mathrm{HT}}t_{\scriptscriptstyle \mathrm{batch}}X^o_{\scriptscriptstyle \mathrm{BHT}}/X^o_{\scriptscriptstyle \mathrm{S}}$	0.25	—	
δ_{13}	$k_{\rm H} t_{\rm batch} X^o_{\rm BH}/X^o_{\rm S}$	0.67	—	
δ_{14}	$k_{ m \scriptscriptstyle HT} t_{ m \scriptscriptstyle batch} X^o_{ m \scriptscriptstyle BHT}/X^o_{ m \scriptscriptstyle S}$	0.61	—	
δ_{15}	$\mu_{ m H} t_{ m batch}$	16.8	—	
δ_{16}	$b_{ m H} t_{ m batch}$	43.0	—	
δ_{17}	$\mu_{ m HT} t_{ m batch}$	24.3	—	
δ_{18}	$b_{ m HT} t_{ m batch}$	5.2	—	
δ19	$(1-Y_{\scriptscriptstyle\rm H})\mu_{\scriptscriptstyle\rm H} t_{\scriptscriptstyle m batch} X^o_{\scriptscriptstyle m BH}/(Y_{\scriptscriptstyle\rm H} S^o_{\scriptscriptstyle m O})$	11.2×10^{3}	—	
δ ₂₀	$(1-Y_{\scriptscriptstyle m HT})\mu_{\scriptscriptstyle m HT}t_{\scriptscriptstyle m batch}X^o_{\scriptscriptstyle m BHT}/(Y_{\scriptscriptstyle m HT}S^o_{\scriptscriptstyle m O})$	16.2×10^{3}	—	
δ_{21}	$k_{La}t_{\rm batch}$	10 ³	—	
δ ₂₂	$\bar{S_{o}}/S_{o}^{o}$	5.0	_	

(3.3) then reduce to

$$\begin{split} \frac{dS_{s}}{dt} &= -\delta_{4} \frac{S_{s}}{\delta_{5} + S_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{\rm BHT} + \delta_{9} \frac{X_{s}}{\delta_{10} X_{\rm BHT} + X_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{\rm BHT}, \\ \frac{dX_{s}}{dt} &= \delta_{12} X_{\rm BHT} - \delta_{14} \frac{X_{s}}{\delta_{10} X_{\rm BHT} + X_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{\rm BHT}, \\ \frac{dX_{\rm BHT}}{dt} &= \delta_{17} \frac{S_{s}}{\delta_{5} + S_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{\rm BHT} - \delta_{18} X_{\rm BHT}, \\ \frac{dS_{o}}{dt} &= -\delta_{20} \frac{S_{s}}{\delta_{5} + S_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{\rm BHT} + \delta_{21} \left(\delta_{22} - S_{o}\right), \\ S_{s} &= 1, X_{s} = 1, X_{\rm BHT} = 1, S_{o} = 1 \quad {\rm at} \quad t = 0. \end{split}$$

$$(3.4)$$

In Figs. 7 and 8, we display numerical solutions of system of equations (3.4) for the parameter values given in Table 5. Comparing these with the solutions given in Figs. 5 and 6, one notes that there is good qualitative agreement and reasonable quantitative agreement, as would be expected.

Motivated by the relevant parameter values listed in Table 4, we denote

$$\delta_5 = \varepsilon, \ \delta_{10} = \theta_1 \varepsilon, \ \delta_{20} = \theta_2 / \varepsilon, \ \delta_{21} = \theta_3 / \varepsilon,$$

where $\theta_1, \theta_2, \theta_3 = \mathcal{O}(1)$, and consider the limit $\varepsilon \to 0$. For reference, it is worth re-displaying equations (3.4) now in terms of the parameter ε

$$\begin{aligned} \frac{dS_{s}}{dt} &= -\delta_{4} \frac{S_{s}}{\varepsilon + S_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{BHT} + \delta_{9} \frac{X_{s}}{\theta_{1} \varepsilon X_{BHT} + X_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{BHT}, \\ \frac{dX_{s}}{dt} &= \delta_{12} X_{BHT} - \delta_{14} \frac{X_{s}}{\theta_{1} \varepsilon X_{BHT} + X_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{BHT}, \\ \frac{dX_{BHT}}{dt} &= \delta_{17} \frac{S_{s}}{\varepsilon + S_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{BHT} - \delta_{18} X_{BHT}, \\ \varepsilon \frac{dS_{o}}{dt} &= -\theta_{2} \frac{S_{s}}{\varepsilon + S_{s}} \frac{S_{o}}{\delta_{6} + S_{o}} X_{BHT} + \theta_{3} (\delta_{22} - S_{o}), \\ S_{s} &= 1, X_{s} = 1, X_{BHT} = 1, S_{o} = 1 \quad \text{at} \quad t = 0. \end{aligned}$$

$$(3.5)$$

The limit $\varepsilon \to 0$ is singular, and the asymptotic structure is indicated in Figs. 7 and 8. We now briefly discuss some of the asymptotic regions (time-scales) arising.

3.3 Region I, $t = O(\varepsilon)$

This very short initial time-scale, which is not even visible in Fig. 7, appears at $t = O(\varepsilon)$ and marks a region of rapid change in the dissolved oxygen concentration. We rescale $t = \varepsilon \hat{t}$, and at leading order we have

$$S_{\scriptscriptstyle \mathrm{S}} \sim 1, \ X_{\scriptscriptstyle \mathrm{S}} \sim 1, \ X_{\scriptscriptstyle \mathrm{BHT}} \sim 1,$$



Figure 7: Plot of the solution to system of equations (3.4) over one day for the parameter values displayed in Table 5. The asymptotic regions for $\varepsilon \to 0$ are indicated.



Figure 8: The same solution as in Figure 7, but plotted over one week. The asymptotic regions for $\varepsilon \to 0$ are indicated.

and pose $S_{o} \sim S_{o}^{I}(\hat{t})$, to obtain

$$\frac{dS_{\scriptscriptstyle O}^{\scriptscriptstyle \rm I}}{d\hat{t}} = -\theta_2 \frac{S_{\scriptscriptstyle O}^{\scriptscriptstyle \rm I}}{\delta_6 + S_{\scriptscriptstyle O}^{\scriptscriptstyle \rm I}} + \theta_3 \left(\delta_{22} - S_{\scriptscriptstyle O}^{\scriptscriptstyle \rm I}\right),$$

where

$$S_{o}^{I} = 1 \operatorname{at} \hat{t} = 0,$$

and $dS_{\rm o}^{\rm \scriptscriptstyle I}/d\hat{t} \to 0,\,S_{\rm o}^{\rm \scriptscriptstyle I} \to \rho_1 \ {\rm as} \ \hat{t} \to \infty,\,{\rm with} \ \rho_1 \ {\rm given} \ {\rm by}$

$$\rho_1 = \frac{1}{2} \left(\delta_{22} - \delta_6 - \frac{\theta_2}{\theta_3} + \sqrt{\left(\delta_{22} - \delta_6 - \frac{\theta_2}{\theta_3} \right)^2 + 4\delta_{22}\delta_6} \right).$$

For the parameter values given in Table 5, $\rho_1 = 0.087$, which is in good agreement with the numerical solution displayed in Fig. 7. We have to note that $\rho_1 > 1$ is also possible, so that the dissolved oxygen is not necessarily depleted over this time-scale; the competing effects of aeration and oxygen consumption by the biomass enter at leading order here.

3.4 Region II, t = O(1) and $t < t_s$

In $t = \mathcal{O}(1)$, we pose

$$S_{\scriptscriptstyle \mathrm{S}} \sim S_{\scriptscriptstyle \mathrm{S}}^{\scriptscriptstyle \mathrm{II}}(t), X_{\scriptscriptstyle \mathrm{S}} \sim X_{\scriptscriptstyle \mathrm{S}}^{\scriptscriptstyle \mathrm{II}}(t), X_{\scriptscriptstyle \mathrm{BHT}} \sim X_{\scriptscriptstyle \mathrm{BHT}}^{\scriptscriptstyle \mathrm{II}}(t), S_{\scriptscriptstyle \mathrm{O}} \sim S_{\scriptscriptstyle \mathrm{O}}^{\scriptscriptstyle \mathrm{II}}(t),$$

for $\varepsilon \to 0$, to obtain

$$\frac{dS_{\rm s}^{\rm II}}{dt} = -\left(\delta_4 - \delta_9\right) \frac{S_{\rm o}^{\rm II}}{\delta_6 + S_{\rm o}^{\rm II}} X_{\rm BHT}^{\rm II},
\frac{dX_{\rm s}^{\rm II}}{dt} = \delta_{12} X_{\rm BHT}^{\rm II} - \delta_{14} \frac{S_{\rm o}^{\rm II}}{\delta_6 + S_{\rm o}^{\rm II}} X_{\rm BHT}^{\rm II},
\frac{dX_{\rm BHT}^{\rm II}}{dt} = \delta_{17} \frac{S_{\rm o}^{\rm II}}{\delta_6 + S_{\rm o}^{\rm II}} X_{\rm BHT}^{\rm II} - \delta_{18} X_{\rm BHT}^{\rm II},
\theta_2 \frac{S_{\rm o}^{\rm II}}{\delta_6 + S_{\rm o}^{\rm II}} X_{\rm BHT}^{\rm II} = \theta_3 \left(\delta_{22} - S_{\rm o}^{\rm II}\right).$$
(3.6)

We do not pursue to solve the system of equations (3.6) here, and confine ourselves instead to considering the system's qualitative behavior. It is clear, that the growth of the biomass is not limited by the availability of S_s , and that hydrolysis is not limited by the availability of X_s . However, both biomass growth and hydrolysis do depend on the available dissolved oxygen here.

From $(3.6)_1$, it is clear that $dS_s^{\scriptscriptstyle II}/dt \leq 0$ for $\delta_4 > \delta_9$, or, in dimensional terms, $\mu_{\scriptscriptstyle HT}/Y_{\scriptscriptstyle HT} > k_{\scriptscriptstyle HT}$. This corresponds to the case of S_s being consumed faster by the biomass than it is generated by hydrolysis. We restrict our discussion here to this case. For this case, there is $t_s = \mathcal{O}(1)$ such that $S_s^{\scriptscriptstyle II}(t_s) = 0$, and this indicates a region that we will discuss next.

3.5 Region III, $t^* = \mathcal{O}(1)$

This time-scale corresponds to $t^* = \mathcal{O}(1)$ where $t = t_s + \varepsilon t^*$, and gives the location of a region where the availability of S_s becomes a limiting factor in the further growth of the biomass. Also, the oxygen concentration undergoes a rapid change over this time-scale. In our numerical solutions (see Fig. 8), $t = t_s$ gives the time when the biomass X_{BHT} achieves its maximum. For $t^* = \mathcal{O}(1)$, we have

$$X_{\scriptscriptstyle \mathrm{S}} \sim X_{\scriptscriptstyle \mathrm{S}}^{\scriptscriptstyle \mathrm{II}}(t_{\scriptscriptstyle \mathrm{S}}), \; X_{\scriptscriptstyle \mathrm{BHT}} \sim X_{\scriptscriptstyle \mathrm{BHT}}^{\scriptscriptstyle \mathrm{II}}(t_{\scriptscriptstyle \mathrm{S}}),$$

where both these quantities are determined as part of the solution to the leading order problem in Region II. In $t^* = O(1)$, we pose

$$S_{\scriptscriptstyle \rm S}\sim \epsilon S_{\scriptscriptstyle \rm S}^{\scriptscriptstyle \rm III}(t^*),\ S_{\scriptscriptstyle \rm O}\sim S_{\scriptscriptstyle \rm O}^{\scriptscriptstyle \rm III}(t^*),$$

to obtain

$$\frac{dS_{\rm s}^{\rm III}}{dt^{*}} = -\delta_{4} \frac{S_{\rm s}^{\rm III}}{1 + S_{\rm s}^{\rm III}} \frac{S_{\rm o}^{\rm III}}{\delta_{6} + S_{\rm o}^{\rm III}} X_{\rm BHT}^{\rm II}(t_{\rm s}) + \delta_{9} \frac{S_{\rm o}^{\rm III}}{\delta_{6} + S_{\rm o}^{\rm III}} X_{\rm BHT}^{\rm II}(t_{\rm s}),$$

$$\frac{dS_{\rm o}^{\rm III}}{dt^{*}} = -\theta_{2} \frac{S_{\rm s}^{\rm III}}{1 + S_{\rm s}^{\rm III}} \frac{S_{\rm o}^{\rm III}}{\delta_{6} + S_{\rm o}^{\rm III}} X_{\rm BHT}^{\rm II}(t_{\rm s}) + \theta_{3} \left(\delta_{22} - S_{\rm o}^{\rm III}\right).$$
(3.7)

As $t^* \to \infty$, $dS_{\rm s}^{\rm \scriptscriptstyle III}/dt^* \to 0$, $dS_{\rm o}^{\rm \scriptscriptstyle III}/dt^* \to 0$, $S_{\rm s}^{\rm \scriptscriptstyle III} \to \rho_2$, $S_{\rm o}^{\rm \scriptscriptstyle III} \to \rho_3$, where

$$\rho_2=\frac{\delta_9}{\delta_4-\delta_9},$$

(recall that we are considering $\delta_4 > \delta_9$ here), and

$$\rho_3 = \frac{1}{2} \left[\delta_{22} - \delta_6 - \frac{\theta_2}{\theta_3} \frac{\delta_9}{\delta_4} X^{\rm \scriptscriptstyle II}_{\rm \scriptscriptstyle BHT}(t_{\rm\scriptscriptstyle S}) + \sqrt{\left(\delta_{22} - \delta_6 - \frac{\theta_2}{\theta_3} \frac{\delta_9}{\delta_4} X^{\rm \scriptscriptstyle II}_{\rm \scriptscriptstyle BHT}(t_{\rm\scriptscriptstyle S}) \right)^2 + 4 \delta_{22} \delta_6} \right]. \label{eq:rho_3}$$

These predictions are in good agreement with the numerical solution displayed in Fig. 7.

3.6 Region IV, $t = \mathcal{O}(1), t_{\rm s} < t < t_{\rm x}$

This is the time-scale over which most of the X_s is degraded. In this region, we have

$$S_{\rm s} \sim \varepsilon \frac{\delta_9}{\delta_4 - \delta_9},$$

and we have $X_s, X_{BHT}, S_o = \mathcal{O}(1)$. For brevity, we do not display or discuss the leading order equations here, and simply note that there is a $t_x = \mathcal{O}(1)$ such that $X_s(t_x) = 0$, which determines the time when the availability of X_s first becomes a limiting factor for hydrolysis.

We omit discussion of Regions V and VI, other than to give their locations and the scalings. Region V is located at $t^{\dagger} = \mathcal{O}(1)$, where $t = t_x + \varepsilon t^{\dagger}$, and in which $S_s, X_s = \mathcal{O}(\varepsilon), X_{BHT}, S_o = \mathcal{O}(1)$. Region VI is at $t = \mathcal{O}(1), t > t_x$ and here we also have $S_s, X_s = \mathcal{O}(\varepsilon), X_{BHT}, S_o = \mathcal{O}(1)$.

4 The ESGI70 Model

The full ASM1 model has large numbers of variables and interactions, and consequently many parameters. The motivation for including these in the model is predominantly microbiological, and seems to arise from the urge to include all possible components about which there is some knowledge. However, many of the parameter values are poorly known: they are dependent on the chemical and microbiological make-up of the particular sludge, and therefore typically used as fitting parameters. With such a highly parameterized model, sets of parameter values can be found to fit most data but it is unclear if the model remains reliable in such situations. Applying a parameterized model under different (but physically reasonable) operating conditions may give spurious modeling artifacts. And this may also cause numerical difficulties in attempting any optimization.

These considerations motivate us to seek a minimal model which should be capable of describing the essential mechanisms of the ATAD process, but ignores issues which — though microbiologically 'known' — are not material to the process within the likely range of operating conditions. It is hoped that such a model might describe the process sufficiently accurately while providing a more suitable basis for optimization.

As indicated in our analysis of the ASM1 model, we opt to ignore the presence of mesophiles since the mixed sludge is hot enough to render their metabolic activity negligible. A biomass concentration variable $X_{\rm B}$ corresponds to the concentration of thermophiles in the sludge. Any mesophiles in the inflow sludge can effectively be considered as already lyzed into additional contributions to substrate and inerts.

We also choose to ignore the distinction between the two pools of substrate S_s and X_s , and consider a single substrate pool X. This is motivated by the urge to simplify to a minimal model, rather than through an assumption that one or other pool may be neglected because it is never rate-limiting under normal operating conditions. The effect of this simplification is greatest after substrate is depleted and becomes limiting (e.g. from Region III of Fig. 7 in the ASM1 model): in our model substrate availability for metabolism is directly dependent on biomass decay, while in the ASM1 model it is buffered by the slow substrate reservoir. The size of this effect remains to be demonstrated as well as its importance in relation to achieving the treatment goals.

For a single batch and a single reactor, we introduce the following governing ordinary differential equations,

$$\frac{dX_{\rm B}}{dt} = G - b(T)X_{\rm B},$$

$$\frac{dX}{dt} = -\alpha G + b(T)(1 - f)X_{\rm B},$$

$$\frac{dS}{dt} = A(\bar{S} - S) - \beta G,$$

$$\frac{dT}{dt} = \lambda G - h(T),$$
(4.1)

where biomass concentration $X_{B}(t)$ has units [g/l], substrate concentration X(t) has units [g/l], S(t) is the oxygen concentration [mg/l], and T(t) is temperature $[^{\circ}C]$. Biomass is assumed here to have a growth rate G given by the dual Michaelis–Menten kinetics expression

$$G = \mu(T) \frac{S}{K_s + S} \frac{X}{K_x + X} X_{\rm B}.$$

$$(4.2)$$

The biomass is also subject to linear decay with rate constant **b** which may be temperaturedependent. Growth of biomass is proportional to the substrate and oxygen consumptions with the consumption efficiency $1/\alpha$ and $1/\beta$ respectively. Substrate X is also produced as a result of decay of biomass, of which a fraction (1 - f) is recycled as substrate.

Dissolved oxygen is replenished through aeration that is subject to the saturation concentration \overline{S} . The sludge temperature increases at a rate proportional to the biomass growth rate and is decreased by heat loss from the reactor. This heat loss occurs through the reactor walls, via the exhaust gas stream from aeration and in the sludge outflow. The heat loss is dominated by losses through latent heat of evaporation in the exhaust gas stream. And while the other heat loss pathways are proportional to $T - T_{amb}$, this heat loss pathway is less temperature-dependent so we model it with a simple constant loss rate.

The parameters for this model are summarized in Table 6. Most of the parameters relate to the thermophile metabolism and sludge properties alone, but those dependent on reactor design are aeration A, heating rate coefficient λ , and heat loss rate h. In the lack of specific plant information, it was deemed appropriate at this stage to focus on operating conditions rather than plant design in any optimization approaches.

This model describes the batch reaction period from just after a batch intake is mixed into the reactor until batch outflow. The required initial conditions are those of the sludge immediately following mixing of the inflow with the sludge remaining in the reactor from the previous batch, since the reactor volume is only partially replaced at each batch. The pre-existing sludge conditions depend on the history of previous batches in the reactor. With repeated batches of the same type, we expect the batch cycle to settle to state in which successive batches are identical and the pre-mixing reactor sludge conditions are effectively independent of the initial conditions of the first batch reactor sludge. We therefore provide initial conditions for the inflow sludge added at each batch and also reactor sludge initial conditions for the first batch. The model can be run to simulate successive batches until these settle to a periodic batch cycle, as

\mathbf{S} ymbol	Description	Value	\mathbf{U} nits	Reference		
Physical parameters						
K _x	half-saturation constant for substrate	0.1	g/l	[1]		
K _s	half-saturation constant for oxygen	0.17	mg/l	н		
μ	growth rate	10	1/d	н		
b	decay rate	5	1/d	н		
α	substrate transformation	1.5	_	н		
β	oxygen transformation	0.5	_	н		
λ	heat production	6.5	°Cl/g	н		
h	heat loss rate	7	°C/d	—		
Ŝ	oxygen saturation constant	10	mg/l	_		
Baseline case parameters						
A	aeration rate	200	1/d	[1]		
$X_{\rm B}^{\rm feed}$	biomass input/feeding rate	1	g/l	н		
$X^{\rm feed}$	sludge input/feeding rate	15	g/l	н		
$S^{\rm feed}$	oxygen input/feeding rate	1	mg/l	н		
$V_{ m in}/V$	ratio of volume input	0.1	—	"		
T^{feed}	temperature of the feed	13	°C	_		

Table 6: Set of parameters for the ATAD model. Some of the units have been converted from their COD (chemical oxygen demand) equivalent.

indicated in Fig. 9. The linking of successive batches and initial mixing of inflow sludge for each batch can be described by adding additional terms into the system:

$$\begin{split} \frac{dX_{\rm B}}{dt} &= G - bX_{\rm B} + Q_{\delta}(X_{\rm B}^{\rm feed} - X_{\rm B}), \\ \frac{dX}{dt} &= -\alpha G + b(1 - f)X_{\rm B} + Q_{\delta}(X^{\rm feed} - X), \\ \frac{dS}{dt} &= A(\bar{S} - S) - \beta G + Q_{\delta}(S^{\rm feed} - S), \\ \frac{dT}{dt} &= \lambda G - h + Q_{\delta}(T^{\rm feed} - T), \end{split}$$

$$\end{split}$$

$$(4.3)$$

where we define the Q_{δ} as

$$Q_{\delta} = \frac{V_{\rm in}}{V} \delta(t - t_{\rm in}),$$

and $\delta(t - t_{in})$ is a Dirac delta function.

The treatment goals for stabilization and pasteurization can be calculated at any solution time after solving the system up to that time. The stabilization target (2.1) is defined in terms of the volatile solids X_{vs} , which can be calculated by integrating

$$\frac{\mathrm{d}X_{\mathrm{vs}}}{\mathrm{d}t} = \mathrm{G}(1-\alpha) + \mathrm{Q}_{\delta}(\mathrm{X}_{\mathrm{vs}}^{\mathrm{feed}} - \mathrm{X}_{\mathrm{vs}}). \tag{4.4}$$

The pasteurization target can be calculated by performing the integration (2.2) while $T > 50^{\circ}C$ and setting L = 0 at other times.

Our first approach is to neglect the temperature dependence of the parameters so that the temperature equation decouples from the system. As typical ATAD operating temperatures are higher than $45^{\circ}C$, we note from Fig. 1 that this will tend to give overestimates of biomass growth and temperature.

4.1 Notes on Optimization

The main operating optimization controls are the aeration rate A, the exchanged volume fraction Q, and the batch reaction time t_{batch} . The inflow sludge properties are largely fixed by the nature of the waste rather than being optimization controls. The exception to this is the possibility of enriching the inflow with additional substrate.

Operational restrictions mean that the aeration rate is generally fixed as constant throughout a batch and the batch time is fixed to give a daily cycle. If we adhere to these restrictions, the controls are reduced to the constant aeration rate A and the exchanged volume fraction Q, and optimization will correspond to the treatment goals being achieved at the end of the daily cycle. In this situation, the energy consumption per mass of treated sludge is proportional to A/Q.



Figure 9: Multiple batch steady-state numerical simulations of the ESGI70-ATAD model.

The effect of aeration rate A is apparently straightforward: additional oxygenation promotes faster biomass growth and therefore quicker stabilization and temperature increase, giving quicker pasteurization. For a fixed batch time and an exchanged volume fraction, we would reduce the aeration rate until the more stringent treatment goal is achieved at the end of the batch. While energy consumption increases linearly with aeration rate, the growth rate's increase with oxygenation is less than linear, approaching linearity near zero oxygen concentration. This would suggest that it may be desirable to maintain the lowest aeration rate which provides sufficient mixing and limits anaerobic metabolism, though other considerations such as plant throughput may become overriding.

The effect of the exchanged volume fraction Q is less clear. The inflow sludge brings new substrate into the reactor, which leads to increased growth rate, digestion, and heating. However, it also cools the sludge mixture which slows the pasteurization process. These two effects have competing impacts on the time to achieve the pasteurization goal. The stabilization treatment goal is expressed in terms of the reduction of volatile solids between inflow and outflow (which is extracted directly from the reactor sludge mixture). Similarly, while inflow brings fresh substrate to fuel the metabolism and promote growth, increasing the exchanged fraction also decreases the apparent stabilization just after inflow mixing which can be expressed as $(1-Q)(1-X_{vs}^*/X_{vs}^{feed})$, where X_{vs}^* relates to the pre-mixing reactor sludge remaining from the previous batch.

A typical ATAD batch reaction follows a timecourse similar to that shown in Fig. 5. The influx of new substrate on initial mixing leads to a rapid increase in metabolic activity and concomitant depletion of oxygen. Substrate is initially in abundance and is digested through the batch reaction, while oxygen is constantly supplied through aeration. At the start of a batch reaction oxygen rapidly becomes limiting while the substrate remains abundant. In this phase the biomass growth rate is mostly determined by the aeration rate and is largely independent of the substrate. As substrate concentration starts to become depleted the control of the process transfers to the diminishing substrate level.

The effect of inflow substrate enrichment is to delay the depletion of substrate, extending the duration of the initial oxygen-depleted phase. It has minimal effect on the growth rate or temperature (and hence treatment goals) until the time at which substrate would otherwise have started to become limiting. As substrate enrichment directly increases inflow volatile solids, it means that a greater quantity of volatile solids must be digested to achieve stabilization.

Once substrate is sufficiently depleted that it is limiting, the oxygen level under constant aeration will generally increase. At this stage, additional substrate comes only from biomass decay (in the ASM1 scheme, via the remaining slow substrate pool), so the growth rate must decrease from this point until decay dominates and then finally the temperature will start to drop. It would therefore appear to continue the reaction (and aeration) significantly into the stage of a decreasing reaction rate except to achieve an unsatisfied treatment goal.

As a broad guideline for optimization, it would therefore appear ideal to adjust the aeration rate and exchanged volume fraction so that the substrate should become depleted close to the end of the batch time, and this should coincide with the two treatment goals being achieved. It is uncertain whether this is achievable with just these controls in a fixed plant design. Increasing aeration accelerates both treatment goals, but directly increases energy consumption. Substrate enrichment enhances pasteurization more than stabilization. Increasing exchanged volume fraction probably delays achievement of both treatment goals, though pasteurization may be greater affected if the post-mixing temperature drops significantly; it also decreases energy consumption by increasing the sludge throughput.

5 Numerical Simulations

The derived model consists of a system of first order ordinary differential equations which are integratated in time using *Matlab's* stiff solver, *ODE15s*. We validate and test the practical applicability of the model by comparing the numerical simulations with experimental data for a specific choice of parameters given in Table 6. A comparison between the experimental data and numerical simulations is given in Figs. 10 and 11 for dynamical operational conditions, i.e., the input volume is not the same for each batch, cf. [2]. Note that here we ignore any temperature dependence of the kinetic parameters. The experiments were carried out under different hydraulic loading which is consistent with the Killarney site, (see for example [8]). Despite the limitations in the available data, the comparison shows a very good fit.



Figure 10: A comparison between experimental data and numerical simulations of the ESGI70-ATAD model for multiple batches.

In the next sections we run the simulations until steady-state conditions are attained. This is done by checking that the solutions between two consecutive batches are within some threshold value. This occurs within 28 days using the baseline case parameters. The numerical simulations for a base case run (and multiple batches) are shown in Fig. 9 where all the parameters are fixed as given in Table 6. Results presented here are for a single reactor and we assume that stabilization is the main goal for bio-treatment. However, for completeness we will also show



Figure 11: A comparison between experimental data and numerical simulations of the ESGI70-ATAD model for multiple batches.

simulations for the case when pasteurization is the main goal. For the purpose of comparison; all simulations are shown for day 28, whether there is stabilization or not, and baseline case simulations are highlighted with a * in the figures.

5.1 Sensitivity to the Feed Temperature, T^{feed}

In this section, we study the sensitivity of the model to variations of feed temperature to investigate the impact of this on the bio-treatment goals, i.e., pasteurization and stabilization. The fresh sludge can be preheated before loading into the reactor using recovered heat. We observe from Fig. 12 that, for the given parameters, stabilization is not sensitive to the feed temperature. However, pasteurization is very sensitive to feed temperature which is consistent with plants with more than one reactor.

5.2 Sensitivity to Sludge Feed, X^{feed}

In this section we consider variations of the sludge feeding pattern to investigate the impact of this on the bio-treatment goals. Fig. 13 suggests the organic feed must be within certain concentrations to attain the required levels of pasteurization and stabilization.

5.3 Sensitivity to Aeration Rate, A

Since there is some uncertainty in the choice of the aeration rate, we run numerical simulations for different values of A. In fact it is an open question whether continuous aeration is necessary



Figure 12: Lethality and stabilization for different feed temperatures.



Figure 13: Lethality and stabilization for different sludge feed concentration.

(such as in the Killarney plant). Numerical results (for a single reactor) suggest that the required treatment goals cannot be achieved for aeration rate lower that $100 \ 1/d$, see Fig. 14.

5.4 Sensitivity to Oxygen Feed, S^{feed}

In this section we consider varying the oxygen feed concentration. We run simulations for values in the range $S^{\text{feed}} = [0.01 - 10] \text{ mg/l}$ and results (not shown here) suggest stabilization and pasteurization are not sensitive to the oxygen feed concentration. This suggests that the plant can operate efficiently at levels lower than $S^{\text{feed}} = 1.0 \text{ mg/l}$ while maintaining the required treatment goals.



Figure 14: Lethality and stabilization for different aeration rates.

6 Optimal Strategy for Pasteurization

In this section we provide an alternative discussion of the optimization problem. We mentioned that the treatment has two different Objectives, namely:

- 1. Killing the pathogen by pasteurization, and
- 2. Stabilization; that is reducing the organic matter contents to an acceptable level (66–80% of the initial).

However, one can expect that when one of these Objectives is achieved, another is already accomplished in the process as well. For example, when the treated sludge is pasteurized and the pathogen are killed or reduced to safe level, this portion of sludge is also already stabilized (that is the organic content is reduced to on acceptable level). This observation allows us to substitute one difficult problem that has two Objectives by two simple separable problems that have a single Objective each. In this Section we consider an optimal control policy that is aimed to pasteurization, assuming that the stabilization will be reached in the process of pasteurizing.

Pasteurization implies exposing the sludge to high temperature for a prolonged time. To achieve this objective in an optimal way, we may consider a simple practical analogue. The optimal policy for pasteurization will be

- 1. Firstly, heat the contents to as high as possible temperature, and do it as quickly as possible.
- 2. After heating, maintain this temperature for the necessary time.

The temperature of the sludge and the heat influx for this process are shown in Fig. 15.



Figure 15: Sludge temperature (given by the curve) and the proposed heat influx (given by the rectangles).

This involved four questions, namely:

Question 1: What is the temperature of the sludge should be?

Answer: The temperature should be as high as it can be maintained for prolonged time. It is obvious that the highest temperature that can be maintained is the temperature when the rate of metabolism balances the bacteria rate of decay (Fig. 16)

Question 2: How long Stage 1 (heating) should be?

Answer: As long as needed to reach the pasteurization temperature at the highest possible heating rate

Question 3: How much heat is needed to maintain the temperature through Stage 2?

Answer: By the model,

$$\frac{d\mathsf{T}}{d\mathsf{t}} = \text{Heat Influx} - \text{Heat Losses.}$$

At equilibrium dT/dt = 0, and hence *Heat Influx* = *Heat Losses*. The heat losses are know for a given temperature, and hence we have the heat influx. For instance, if the heat losses are linearly proportional to the temperature, that is Heat Losses = hT, and the heat influx is proportional to the rate of metabolism,

$$\mathrm{Heat}~\mathrm{Influx} = \mu \frac{S}{K_s + S} \frac{X}{K_x + X} X_{\scriptscriptstyle\mathrm{B}}$$



Figure 16: The equilibrium of the metabolism rate and the rate of decay.

then the task is to maintain the oxygen concentration S at such a level that

$$\frac{S}{K_s+S}\approx 1.$$

Question 4: How long Stage 2 should be?

Answer: As long as needed to reach the required level of pasteurization (this time is well known and is given by a know formula).

6.1 Recommendations

- 1. Thermal-isolation and utilizing the waste heat. Thermal-isolation reduces heat losses and hence the heat influx can be also reduced.
- 2. Splitting the process by stages. We suggest that the process should be divided into two stages, namely the heating and the maintaining the temperature. It is advisable to conduct these two processes in different reactors.
- 3. Preheating the water (utilizing waste heat). Preheating the water would shortening the first stage, the heating and the thermal shock will be smaller.
- 4. Start every round of the process at the highest possible initial concentration of bacteria. This again should shortening the first stage (the heating) and hence reduce the energy losses..

7 Concluding remarks

During the 70th European Study Group, the participants mathematically addressed a problem of optimizing the process of waste water bio-remediation. It was noted by the participants that the models that currently exist are greatly oversized, while the reliable data are rather scarce. Furthermore, it was also noted that the existing models are very sensitive to the parameter values. It was suggested, therefore, that under the circumstance a simpler model is needed.

Such a model, that includes only the essence of the process, has been developed during the Study Group. This model includes four crucial variables, namely the substrate concentration (the nutrient), the biomass, the oxygen concentration and the temperature of the sludge. The model describes the process of bio-treatment for the case of a single reactor. It has been shown, that for correctly re-calibrated parameters the ESGI model and the original large-scale models give effectively the same outcome. Development and verification of this model was the major outcome of this study. An extension of this model to the case of a few sequential reactors is reasonable straightforward and possesses no difficulty.

In the analysis that are presented in this report, we applied this model to consider two different regimes, namely, when either oxygen, or the substrate (the nutrient) are limiting factors. It appears that one possible operating strategy can be applying a low aeration rate to preserve the oxygen concentration a limiting factor for longer, with the aim that the two objective of the bio-treatment were met at the same moment at the end of the cycle.

We would also like to remark that the participant realize that the problem of optimizing of the bio-treatment, as it was presented to the Study Group, is essentially a problem of optimal control. However, taking into consideration that the problem is fundamentally non-linear, addressing this optimal control problem analytically is a highly non-trivial task. This problem in such circumstances may be explored numerically, applying the technique that is known as dynamic control. However, a reliable and reasonably simple model is needed for this at the first instance, and we believe that the model that was developed can serve as the basis for such study.

Study of the model also gives an important insight into the nature of the process, and enables us to gain a number of practically relevant recommendations. Thus, it appears that pre-heating the input sludge will be beneficial, provided it can be done in an energy efficient way (recycling the wasted heat that is generated in the process).

One avenue for further research is an extension of the ESGI70 model to reactors in series. This study would be of assistance for a more complex physical plant design.

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