Grundfos: Chlorination of Swimming Pools

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1 Introduction

Grundfos asked for a model, describing the problem of mixing chemicals, being dosed into water systems, to be developed. The application of the model should be dedicated to dosing aqueous solution of chlorine into swimming pools.

The first thing to be decided is the type of model we are looking for; in particular whether this is a diffusion dominated problem (where spatial gradients and diffusion times are important) or a sink-source type of ordinary differential equation problem like the CSTR (Continuously Stirred Tank Reaktor).

Swimming pools as a rule are designed specifically to mix the re-circulated water well, i.e., much faster than the typical diffusion time associated with the pool size. Such a rapid mixing is accomplished by having the chlorinated water re-enter the pool through a large (30–80) number of jets, evenly spaced across the pool bottom. The actual mixing time in a particular public pool is monitored as a part of the routine whenever the pool water is to be drained prior to a filling with fresh water.

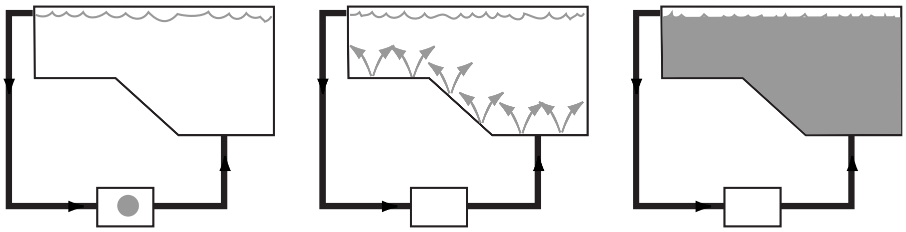

Figure 1: Mixing jets at bottom of pool.

As the final operation on the 'dirty' water, a single blob of dye is injected into the water entry system, and the subsequent spreading of the dye throughout the pool is observed and timed, see figure 1. A well functioning jet system (such as e.g., in the *Lyngby Svømmehal*) mixes the dye evenly in the entire pool in 2–3 minutes; a mixing time of less than 10 minutes is required by law in Denmark. The observed mixing time of 2–3 minutes, is far less than the diffusion time associated with pool size.

The conclusion is that, on the time scale of interest (i.e., hours), setting $\frac{\partial}{\partial x}$, $\frac{\partial}{\partial y}$, and $\frac{\partial}{\partial z} \approx 0$ is a good approximation. The pool indeed resembles the CSTR model, and can for the present purpose be modeled by a system of ordinary differential equations.

2 An ODE Model

We introduce three variables denoting the (approximatly) uniform concentrations of the following quantities:

$c(t)$ = concentration of 'free' chlorine ($ClOH$) [moles/l]
$b(t)$ = concentration of bacteria [10^9 parts/l]
$p(t)$ = concentration of organic pollutants [moles/l]

Three coupled ODE's for the time evolution of these quantities are to be set up, with source and sink terms. We begin with sources and sinks for the chlorine.

2.1 Chlorine sources and sinks

The pump and its reservoir of chlorine is a source term. The pump is connected to a chlorine gauge near the pool overflow channel, and the pump injects well separated doses of chlorine with a variable stroke frequency, i.e., a stroke rate that depends on the chlorine concentration. Figure 2 displays the stroke frequency R as a function of the concentration c.

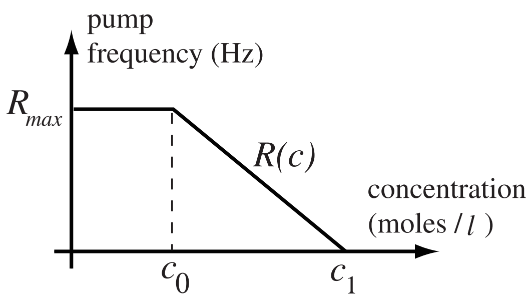

Figure 2: Chlorine injection strategy.

When the chlorine concentration is above a value c_1, the pump is off. Below c_1, the pump frequency increases linearly with decreasing c until at c_0 a maximal pump frequency R_{max} is reached. This feedback strategy will be referred to as *the ramp*, for obvious reasons. The functional form of the source term in the equation is consequently $G/V \cdot R(c)$, where

$$R(c) = \begin{cases} 0 & \text{if } c_1 < c \\ R_{max} \frac{c_1 - c}{c_1 - c_0} & \text{if } c_0 < c < c_1 \\ R_{max} & \text{if } c < c_0 \end{cases}$$

where V is the total volume of the pool, and the constant G denotes the dosage per stroke. We use a value for $G \cdot R_{max}$ of 30 moles/hour.

Next, we discuss the loss mechanisms for the chlorine. The first one of these is the chemical reactions that bind chlorine with the organic polutants p. We assume that this is a first-order chemical reaction,

$$cl + p \rightarrow clp$$

with rate constant k_4, such that the loss term is

$$-k_4 c(t) p(t)$$

The value of rate constant k_4 will be a parameter in the model.

We must also estimate the loss of chlorine due to its reaction with bacteria.

Not much is known at the microbiological level about the details of the process by which bacteria are killed by chlorine. The interaction with one molecule of chlorine is probably not enough to kill one bacteria. With the concentrations involved in the present study, there are 10^{27} chlorine molecules and 10^{10} bacteria. Even if it takes 1000 molecules of chlorine to eliminate one bacteria, the concentration of chlorine will not affected measurably.

Based on this consideration we make the assumption in this report that the chlorine kills the bacteria without actually depleting the chlorine concentration. Hence there will be no bacteria dependent sink term in the chlorine equation.

Alternativly, one could model (but this is not done in the present treatment) the bacteria as amorpheous lumps of molecules, all of which eventually react with the free chlorine to stable compounds. The details of such a reaction, the stoechiometry as well as the time scales for the various reactions, would be appropriate for models more detailed than the one considered here.

Finally, we consider the 'physical' loss of chlorine due to the filters through which the pool water is circulated, due to evaporation, or to migration into pipes and walls. This is taken to be a slow, zeroth order process, with a rate constant which we estimate from observations of the chlorination needed to maintain a constant $c(t)$ when no bathers are present (e.g., over night, or when the pools are closed to bathers for other reasons). The appropriate term has the form:

$$-k_1 c(t)$$

A typical value of k_1 is estimated from actual pool data [5]. If, in order to maintain concentration, an amount corresponding to 1/4 of the total amount of chlorine present needs to be added after a 24 hour period (with no other sink term being present) the rate constant must have a value of about $k_1 = 0.01\mathrm{h}^{-1}$.

2.2 Source and loss terms for p

The quantity p originates with the bathers [1]. In this model, each bather is assumed to stay in the pool for one hour, and in this hour to deposit roughly 5 grams of organic molecules of fairly large molecular weight (100 - 500 g/mole). See [1], p. 285. Let $N(t)$ = # of people in the pool as a function of time (i.e., throughout the day), then the source term is

$$\frac{\alpha}{V} N(t)$$

where $.01 < \alpha < .05$. In this study, we took as a specific $N(t)$ a simple sinusoidal variation throughout the day, and zero at night:

$$N(t) = \begin{cases} 80 \sin^2\left(\frac{\pi}{2} t\right) & \text{if } 0 < [t]_{24} < 12 \\ 0 & \text{otherwise} \end{cases}$$

see figure 3. A loss term for quantity p is the reaction with the free chlorine to form the compound cp:

$$-k_4 cp$$

Such a term also appears in the chlorine equation, and as already stated, the value of k_4 is regarded as a free parameter in the present model.

[1] No, the letter for this variable was not chosen arbitrarily.

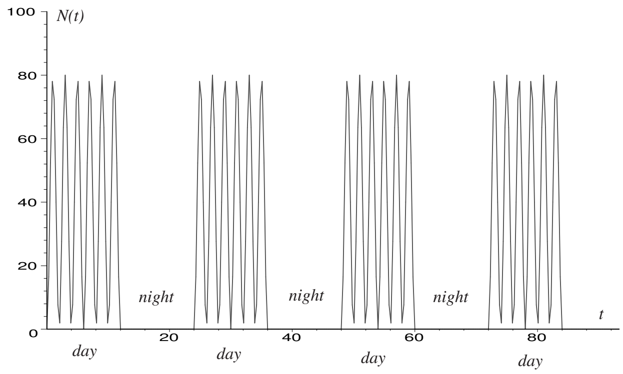

Figure 3: The assumed time dependent number $N(t)$ of bathers.

2.3 Source and loss terms for b

Bacteria are also deposited by the bathers. It is estimated [1] that each bather deposits about 10^8 bacteria per liter per hour. The source term for b is consequently

$$\beta N(t)$$

where $\beta \approx 0.1 \times 10^9/\mathrm{h}$. Furthermore, bacteria are live and will grow by themselves (feeding off salts and and organic substances in the pool) unless kept in check by the chlorine; this process is described in the following source term for b:

$$k_3 b(t)$$

where a worst-case scenario (a two-hour doubling time) would correspond to a value for k_3 on the order of $1/3\mathrm{h}^{-1}$.

In spite of the fact that we did not take bacteria as a loss term for chlorine, we do take chlorine to act as a loss term for bacteria; kinetically as a first-order reaction:

$$-k_2 c(t) b(t)$$

We estimate from data reported [3, 4] that the rate constant has a value of about $k_2 = 8 \times 10^6 l/(\mathrm{mole\ h})$.

In principle, there is one further loss term associated with the number of bacteria themselves (due to overpopulation and deplection of nourishment, as in 'predator-prey' models). But the numbers of bacteria will (hopefully!) never get so large that this term becomes significant. So we leave it out from the b equation.

3 The ODE system

Collecting all the source and loss terms of the pervious section into a system of Ordinary Differential Equations, we have:

$$\begin{aligned} \frac{dc}{dt} &= \frac{G}{V} R(c) - k_4 c p - k_1 c \\ \frac{db}{dt} &= \beta N(t) + (k_3 - k_2 c)\, b \\ \frac{dp}{dt} &= \frac{\alpha}{V} N(t) - k_4 c p \end{aligned} \tag{1}$$

where

$$\begin{aligned} GR_{max} &= 30 \text{ moles/ h} & V &= 8 \times 10^5 \; l \\ k_1 &= 0.01 \text{ h}^{-1} & k_2 &= 8 \times 10^6 \text{ l/(mol} \cdot \text{h)} \\ k_3 &= 1/3 \text{ h}^{-1} & \alpha &= 0.01 \to 0.05 \text{ moles/(pers.} \cdot \text{h)} \end{aligned}$$

Note that we have no set value for k_4. This rate constant describes in this model the rate at which chlorine is consumed by reaction with with the p quantity, and vice versa. In a more detailed model, more variables coupling through more chemical reactions might give a more detailed view. Here, with just a single coupling, we examine the qualitative changes in the evolution of the substances c, b, and p over some days, as k_4 is set to values with different orders of magnitude. Specifically, we shall examine the solutions at parameter values $k_4 = 50$, 500, 5 000, and 50 000.

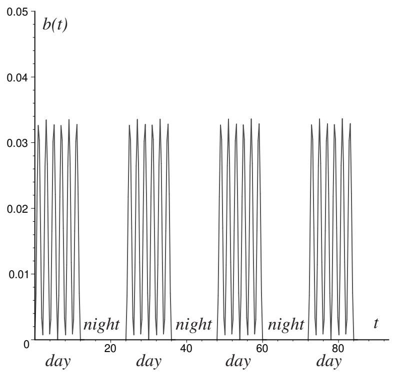

Figure 4: The time evolution of b for all examined values of k_4.

The variable b is found in this model to have an evolution that is nearly independent of such a variation in k_4. The quantity is input (via the bathers), and destroyed rapidly by the chlorine; at the end of each day, nothing remains.

This is not the case for the time evolution of the variables c and p, as illustrated in the figures below.

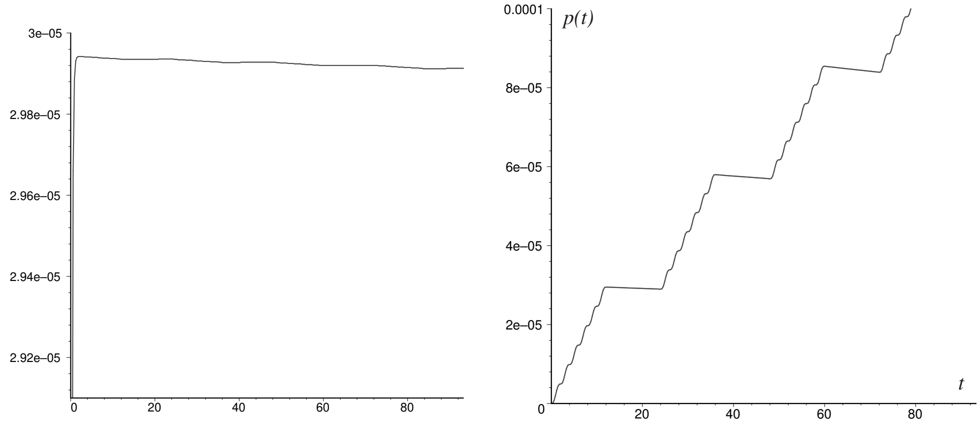

Figure 5: c(t) and p(t) for $k_4 = 50$.

For the lowest examined value of k_4, we find that c increases rapidly until a saturation value of just under 3×10^{-5} moles$/l$ is reached. This is a value where the pump input balances the 'background' loss of c. The p quantity is cumulatively added by the N function, and the $c - p$ reaction rate does not, at least on the time scale of a few days, have any influence on the accumulation of p. (only the slowly decreasing saturation level of c indicates in figure 5 that there is a $c - p$ reaction at all).

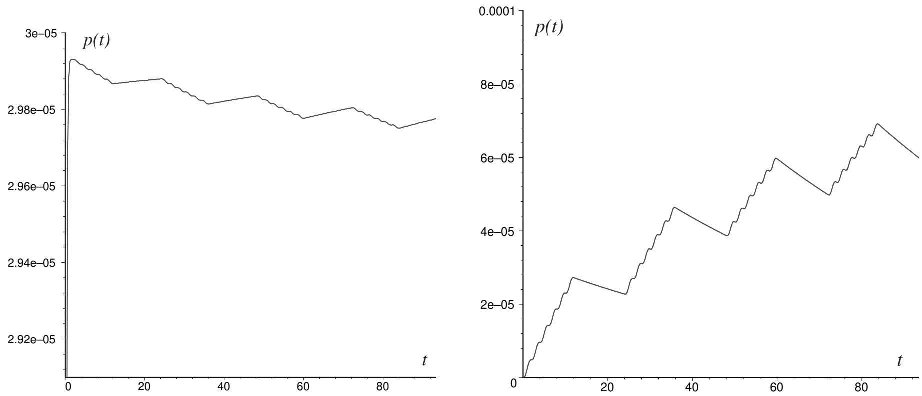

Figure 6: $c(t)$ and $p(t)$ for $k_4 = 500$.

For a ten times higher value of k_4 (see figure 6), the effect of the reaction on the chlorine level begins to be detectable; from its initial saturation level, the daytime loss of c is followed by night time return towards a saturation level. The slow decrease over a time scale of days is now more pronounced. The effect of the higher k_4 value on the p evolution is that at night the p, instead of remaining nearly constant, now is slowly being depleted by the $c - p$ reaction; but the daytime load still 'wins', and over a time scale of days the p accumulates, though possibly with an upper bound.

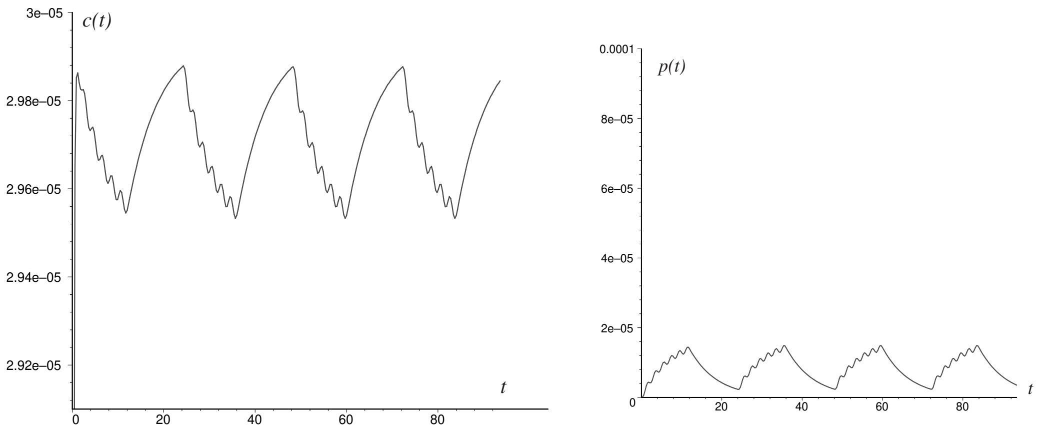

Figure 7: $c(t)$ and $p(t)$ for $k_4 = 5000$.

In figure 7, for $k_4 = 5000$, the $N(t)$ induced oscillations are quite pronounced, and the $c - p$ reaction term at this parameter value influences the solution significantly. The daytime $N(t)$-oscillations can be detected in the decreasing part of the curve. At night, the ramped pump function drives the c level up towards the saturation level, but before a steady state is reached, morning arrives, and more bathers. Nevertheless, the overall c variation on a time scale of several days is at the percentage level, a fluctuation which is acceptable by current standards.

The p evolution curve at this value of k_4 is qualitatively different from the previous two; it no longer shows a long term accumulation. Over the time scale of a single day there is a build-up, but at night the $c - p$ reaction drives the level back down; a constant average level seems to be maintained.

Finally, we can see in figure 8 the effect of a ten times higher value, $k_4 = 50.000$. The daily oscillations now take place around a lower average c value (however: note the scale, the variation is still at the percentage level). The nightly saturations with c run more nearly to completion.

The p level is now very low (we have maintained the same scale as in previous figures, for comparison), and does not show any tendency to accumulate at all. This value of the reaction constant very effectivly keeps the p level in check.

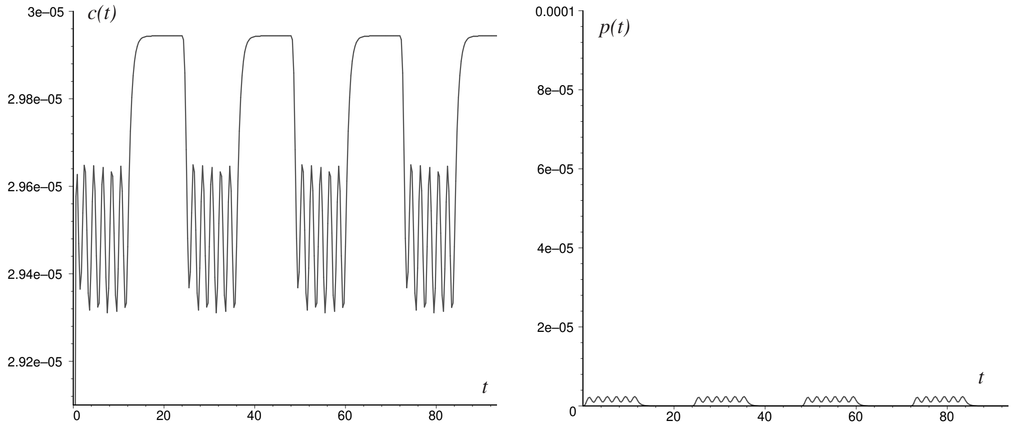

Figure 8: $c(t)$ and $p(t)$ for $k_4 = 50.000$.

4 Discussion

The chemistry in swimming pools is of considerable complexity [1, 6]. The above considerations constitute the simplest model, so to speak, in the chemistry. It contains the minimal number of variables: chlorine, one organic (b) pollutant, one inorganic (p) pollutant, and the very crudest sink, source and interaction terms for these quantities.

In particular the higher order reactions between chloride and ammonia are certainly of interest in a more detailed study, as the end compounds are potentially carcenogenic and hard to remove by filters.

Furthermore, various types of pump strategies (e.g., other response functions than the ramp) might be examined. In our opinion, the qualitative conclusions arrived at here will be invariant for a large class of ramp-like functions, but this of course should be tested.

5 Summary

We have determined that, consistent with the engineering design of pools, fluid mixing is so rapid that the time evolution of chemicals and bacteria in a pool system is well modelled by a set of coupled ordinary differential equations (ODE's).

We have constructed, as a simple model, a 3-variable ODE system, containing the evolution and coupling between one variable representing the chlorine concentration, one variable representing the concentration of bacteria, and one variable representing the concentration of organic molecules.

This model indicates that, with the chlorine as the only means to remove the organic pollutants supplied by the bathers, the rate at which the organic substances accumulate has strong dependence on the chemical reaction constant k_4. At sufficiently high values of k_4, the concentration of organic pollutants does not accumulate, on the time scale of interest.

The explicit pump strategy examined (the 'ramp') is effective in regulating the chlorine concentration.

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LEGO: Automated Model Construction

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1 The Problem Description

The question from LEGO was, “Given any 3D body, how can it be built from LEGO bricks?”

We will assume that we have a “legoised” model, i.e., a 3D matrix containing ones in the places where unit-volume LEGO bricks should be put and zeros where there should be empty spaces. A LEGO unit-volume is a brick 8 mm long and wide and 3.2 mm high which has only one stud on the top for connection with other bricks.

So the task was to make an algorithm which takes as its input a legoised 3D model and produces a way of constructing the model from actual LEGO bricks so that the model “stands” connected.

We were restricted to the use of so-called “family” LEGO bricks and LEGO DUPLO bricks. Both kinds are rectangular prisms whose dimensions in each direction are integer multiples of the unit LEGO brick's dimensions. The lengths, widths and heights of bricks are measured quite naturally in terms of unit bricks. We were given a table of sizes of all the permitted building blocks. Due to the construction of LEGO DUPLO, these bricks can be connected to family bricks with even length and width only. Another restriction is that only family bricks of height 3 or more can be connected to the top of a DUPLO brick.

As there is more than one way of building any model of even quite small size LEGO suggested that we should seek “more stable” models. More stable models are those which are made with bigger bricks and with bricks that have more studs connected to other bricks.

Nothing can be assumed about the shape of a legoised object given as input except that it is connected. However, some characteristics of typical models and how they are commonly built were discussed.

If a model is of sufficiently large size then its interior should have a hollow space in order to save bricks. LEGO designers keep this space approximately box-shaped for simplicity and so that a supporting structure or motorised mechanism can be placed there if necessary. The thickness of the shell of such a hollow structure is between 2 and 6 unit bricks at its minimum. Faced with the task of building such a model, LEGO builders construct it roughly layer by layer. They start with a small area including part of the visible outer edge, then they work on the inner edge, that of the hollow box which is interior to the model, and finally they fill in the area between the outer and inner walls.

We found out that some "cheating" is even allowed when building a LEGO model. That is to say, one may alter the model by very small amounts if the change produces a model which still "looks good" and the change is beneficial in some other way, for example if it increases the stability.

At a later stage LEGO would like to incorporate the use of different coloured bricks, so our automated building technique should take that into consideration.

The only other requirement was that the algorithm would produce a result within a few days and thus does not need to run for enormous amounts of time to get an answer. LEGO is interested in the solution of the problem for relatively large models as are used in their parks or at exhibitions for advertising purposes. These models are typically made from approximately one million bricks. Of course, the legoised versions of these models would have a far greater number of unit LEGO bricks — the number could be expected to be at least an order of magnitude greater. In these circumstances running time is extremely important.

2 The Simplified Approach

The LEGO problem is a huge and complicated problem so in the first instance it was necessary to simplify it.

Although the use of DUPLO bricks is desirable as building with them is both cheaper and quicker, we restricted ourselves to the use of one height of brick only, the common brick of height equal to 3 minimal LEGO units. In this way we could concentrate on building layers in the model, one at a time, without concern about any brick being in more than one layer at a time. However, any algorithm which can work for bricks of height 3 could be applied without any problems to bricks of other heights if all bricks in any one layer were of uniform height. It would require some work to create an algorithm to accept bricks of mixed heights and that was beyond the scope of the study group work.

Another assumption we made was that the shape of the inner hole was given by the legoisation and we were to keep the size and shape of the legoisation regardless of the price. The reason is that to take into account what kind of "cheating" may be allowable would increase the problem size tremendously.

One layer of a model with an inner hole might look as in Figure 1.