Population Balance Models: A useful complementary modelling framework for future WWTP modelling

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Abstract
Population Balance Models (PBMs) represent a powerful modelling framework for the description of the dynamics of properties that are characterised by statistical distributions. This has been demonstrated in many chemical engineering applications. Modelling efforts of several current and future unit processes in WWTPs could potentially benefit from this framework, especially when distributed dynamics have a significant impact on the overall unit process performance. In these cases, current models that rely on average properties cannot sufficiently captured the true behaviour. Examples are bubble size, floc size, crystal size or granule size,... PBMs can be used to provide new insights that can be embedded in our current models to improve their predictive capability. This paper provides an overview of current applications and the future potential of PBMs in the field of WWT modelling, introducing new insights and knowledge from other scientific disciplines.

INTRODUCTION TO POPULATION BALANCE MODELS (PBM)

Many natural systems consist of populations of individual entities (e.g. flocs, bubbles, granules, crystals, bacterial cells) with specific properties (e.g. size, composition, density, activity). The individual entities interact with their environment (e.g. dissolved chemical precipitation, oxygen transfer from air bubble to liquid phase, shear-induced breakup) or with one another (e.g. aggregation, coalescence). Typically, these interactions are a function of one or more properties, which may vary within a population of entities. In this context, we can refer to this variation as "distributed properties" as they can be represented by a distribution instead of a scalar (i.e. one single value). A simple example of the use of a distribution would be to characterize the variation in floc size in an activated sludge system. This distributed feature implies that the behaviour of distinct entities can be significantly different, and can deviate substantially from 'average' non-distributed behaviour.

Current modelling frameworks usually assume non-distributed scalar properties (e.g. using a single particle size or bubble size), implying that all individuals behave in exactly the same way. In some cases, this is sufficient, but in others this assumption is too strict and will lead to predictions that deviate significantly from the real system. The required level of detail is clearly governed by the modelling objective. Yet, few researchers and design engineers in WWT are aware of alternative modelling approaches that can account for the impact of these distributed properties on unit process performance.

A framework to achieve distributed behaviour by considering distributed population properties already exists and is called Population Balance Models (PBMs). PBMs have been

extensively used in chemical engineering for a myriad of applications (Ramkrishna, 2000; Marchisio, 2012). The governing equation in its most general form is given as

$$\frac{\partial f_1(x,t)}{\partial t} + \frac{\partial}{\partial x}\left(\dot{X}(x,t)f_1(x,t)\right) = h(x,t) \qquad \text{Eq. 1}$$

where x is the internal coordinate (i.e. the distributed property), $f_1(x,t)$ is the number density function (i.e. the distribution of the distributed property), $\dot{X}(x,t)$ is the continuous growth term of x and $h(x,t)$ is the PBM reaction term (through discrete events). Table 1 provides some examples in regard to wastewater treatment applications.

Table 1 – Some examples of wastewater treatment processes and related internal coordinates (x), number density functions ($f_1(x,t)$) and continuous ($\dot{X}(x,t)$) and discrete ($h(x,t)$) governing mechanisms

Process	X	$f_1(x,t)$	$\dot{X}(x,t)$	$h(x,t)$
(De)flocculation*	Floc size	Floc size distribution	Microbial growth	Aggregation, breakage
	Size/Density**	Size/Density distribution	-	Aggregation
Coalescence	Bubble size	Bubble size distribution	-	Coalescence
Granulation	Granule size	Granule size distribution	Microbial growth	Granulation
Crystallization	Crystal size	Crystal size distribution	Crystal growth	Aggregation, breakup
Bio P-removal	Poly-P	Poly-P distribution	Poly-P storage, release	Cell division, cell birth
PHB production	PHB	PHB distribution	PHB storage, release	Cell division, cell birth
Growth	μ_{max}	μ_{max} distribution	Growth rate gradient	Cell division, cell birth
Affinity	Kx	Kx distribution	Affinity gradient	Cell division, cell birth

*Note that this mechanism is driving the settling processes in primary and secondary sedimentation
**In this case a 2D PBM is obtained

The first term on the left hand side of Eq. 1 represents the accumulation term. Distribution dynamics that can be described are either governed by continuous processes (e.g. biomass growth, crystal growth, particle drying – represented by the second term on the left hand side of Eq. 1) or discrete processes (e.g. aggregation, breakage, coalescence, granulation – represented by the term on the right hand side). The latter term usually consists of a birth and a death term, where the birth rate describes the rate at which particles of property x are being formed and the death rate describes the rate at which they are being removed. In crystallisation, a nucleation term needs to be added in the smallest size class mimicking the nucleus that is formed in an oversaturated solution.

The internal coordinate x can be either a scalar (i.e. a single independent variable) or a vector resulting in a 1 dimensional or multi-dimensional PBM, respectively. The use of multi-dimensional PBMs means that the distribution of one or more material properties can be described. It should be noted that formulating and solving multidimensional PBMs is a challenging task.

The nature of the resulting equation depends on the presence of the $\dot{X}(x,t)$ and $h(x,t)$ terms. If only the former is present, a partial differential equation (PDE) is obtained for which solution methods are available. The latter term usually contains integral terms expressing the interactions between members of the distribution, turning the equation into an integro-partial differential equation. Several numerical methods have been reported in the literature to solve this type of equations (Ramkrishna, 2000).

Applications of PBMs to wastewater treatment processes are rather scarce. The first application was introduced by Fukushi et al. (1995), where a PBM model was used for modelling the dissolved air flotation process in water and wastewater treatment. The authors described the attachment process of bubbles to flocs during the flocculation process in a turbulent flow. Gujer (2002) investigated the impact of lumped average cell composition versus distributed composition in the context of ASM2 and ASM3 and concluded that this indeed had a significant impact. Schuler (2005) demonstrated that lumped state (= averaged) assumptions in EBPR system performance models produced large errors due to the difference in individual residence times of organisms in different zones. This was found to be related to process hydraulics (Schuler, 2006) and to impact the endogenous respiration as the latter was found to be more important when distributed models were applied (Schuler and Jassby, 2007). Finally, several PBM references can be found in the field of activated sludge flocculation ranging from very simple formulations (Parker et al., 1972) to more elaborate ones (Biggs et al., 2003; Nopens et al., 2002) and papers focussing on experimental validation (Nopens et al., 2005) and model structure analysis (Nopens et al., 2007; Torfs et al., 2012).

PBMs can serve the purpose of building process understanding. The result of such a detailed modelling exercise can be included in next generation simplified WWTP models that go beyond the currently used paradigms (i.e. ASM using averaged biomass behaviour combined with residence time distribution models and oversimplified aeration and settling models). Hence, PBM models should not be considered as replacement of current WWTP models, but as enhancement tools to improve the future quality of their unit process predictions. This paper intends to outline the potential of PBMs in the field of wastewater treatment through several examples of different WWTP unit processes.

APPLICATIONS OF PBMS IN THE FIELD OF WWT

Improved flocculation to better exploit primary and secondary settling
The current settling models are either based on removal efficiencies or settling velocities correlated with particle concentration. Settler models are still receiving attention as there is still room for improvement in their use (e.g. storage function during wet weather) and operation. This is especially true for primary settlers as they can be an important asset for energy recovery through the maximisation of the primary sludge that is sent to the anaerobic digester. Their behaviour has not been widely studied thus far (Bachis et al., 2014). Moreover, the primary treatment process is often chemically enhanced (CEPT) which creates an optimal dosage problem. As particle concentrations are low in primary settlers, the settling regime is not hindered but rather discrete, i.e. Stokian, and a function of particle size, shape and density, leading to a wide distribution of settling velocities as evidenced by Bachis et al. (2014). The discrete settling assumption is also true for the zone just above the sludge blanket of a secondary settler. In discrete settling, settling velocities are directly related to size, shape and density and, hence, the particle size distribution (PSD). The PSD depends on the original flocculation state as well as on actions undertaken to improve the flocculation state (e.g. turbulent shear, coagulant). Note that the flocculation state also depends on the particle's history (e.g; a sludge can have the same PSD, but it can react very different if the floc strength is different caused by a different flocculation history).
Flocculation of particles is probably the most straightforward application of PBMs. Since biological growth occurs on a much longer time scale compared to aggregation and breakage

it can be ignored when studying short-term flocculation behaviour of activated sludge. The PBM reaction term is then defined as

$$h(x,t) = B(x)_{agg} - D(x)_{agg} + B(x)_{break} - D(x)_{break}$$ Eq. 2

in which the birth (B) and death (D) terms occur for both aggregation and breakage as shown in Figure 1. Through these different mechanisms flocs of any size can be formed or removed. Furthermore, it becomes clear that aggregation is a particle-particle interaction process, whereas shear-induced breakage is not. The rates of all these processes are, hence, governed by the number of flocs present (N) as well as an aggregation rate (β), an aggregation efficiency (α) and a breakage rate (S) and distribution of resulting particles (the so-called daughter size distribution). Aggregation and breakage rates are in their turn a function of the mechanisms that drive the aggregation or breakup. Traditionally, shear and polymer addition are accounted for which is likely sufficient for the application in the context of primary and secondary settling. More details on these rates and their dependencies on shear and flocculant addition can be found elsewhere (Nopens et al., 2002; Nopens et al., 2005). An example of a model prediction along with measured size distribution during a batch sludge flocculation process is shown in Fig. 2.
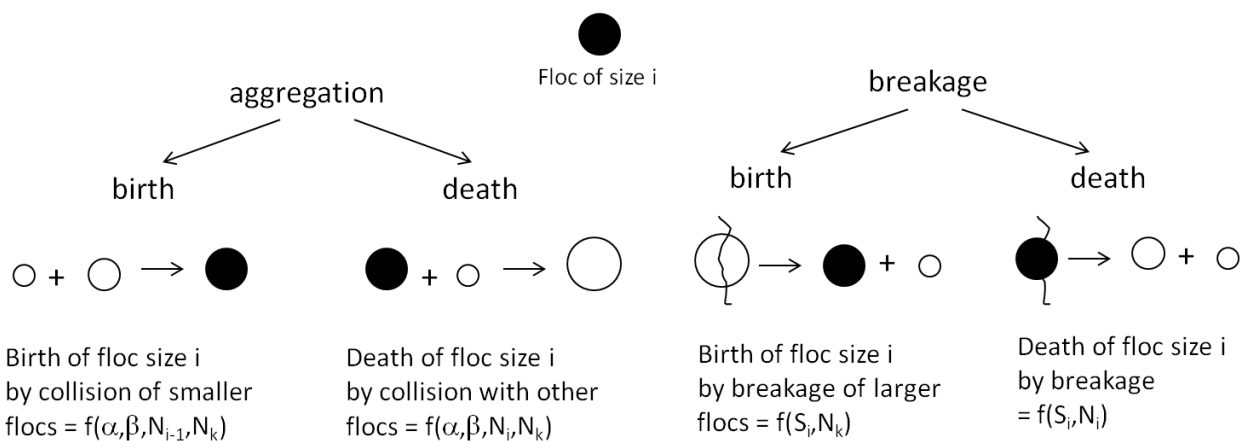

Fig. 1 – Illustration of mechanisms involved in flocculation (after Nopens et al., 2002)
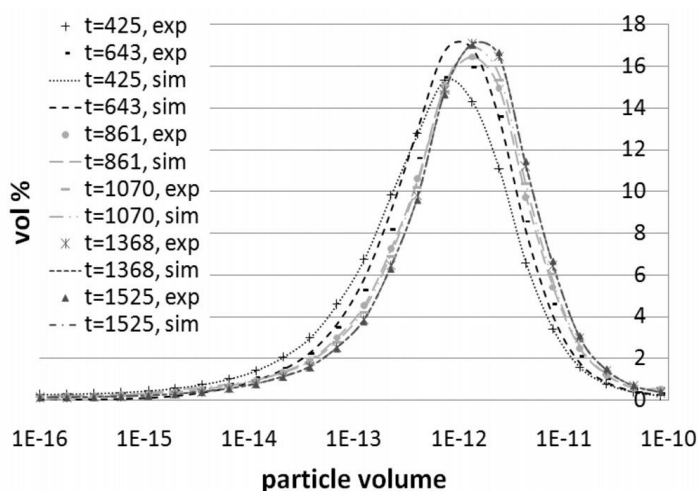

Fig. 2 – Example of a PBM model prediction of a batch sludge flocculation process (time unit = seconds; unit on size axis = μm^3) after Torfs et al., 2012)

Flocculation usually takes place in the process units prior to the actual settling tank as well as in the settling tanks (if conditions are good). Flocculation models as described above can be used for both. Currently, the flocculation process in primary and secondary clarifiers is not studied in detail and its effects are incorporated using rules of thumb. However, understanding the contribution of flocculation would improve their design and operation which can significantly improve the settling performance and control. Indeed, being able to predict and control the size distribution of a population of particles arriving to either the primary or secondary settler would be a useful input to settler models that can handle a distribution of settling velocities, calculated from the size distribution derived with the PBM (Bachis et al., 2014).

In a secondary settler, exposure of flocs to elevated shear during transport from the bioreactor to the centre well of the settler will induce reflocculation and impact the floc size distribution and the floc strength. An appropriate application of PBM for settler induced flocculation would specify size as the internal coordinate.

In primary settler applications, the availability of particle settling velocity distributions as the internal coordinate of the suspended solids has generated a more accurate prediction of the load to the secondary treatment model, reduced the need for calibration (Bachis et al., 2012, 2014), and produced more accurate and optimal control of chemical dosage that lead to cost savings. In addition to particle size, particle density can be included as a second internal coordinate when density varies significantly with floc size. This additional internal coordinate can be accomplished using a 2D PBM approach but comes with an increased computational and parameter estimation cost since the rate expressions need to be extended to include density, which will require a detailed investigation of the process. Another interesting route for further research is the coupling of PBMs to computational fluid dynamics models as the latter can predict local shear which then serves as input for the PBM model. Research that couples PBM with CFD in WWT has been reported already (Griborio et al., 2006; Gong et al., 2011), but needs further attention. Here, again, it should be clear that coupling a 1D PBM to a CFD model is a challenging task, typically resulting in models which need very long simulation times. One strategy to reduce the computational burden is to reduce the PBM model before coupling it to a CFD model (Mortier et al., 2013).

More accurate aeration modelling for better design and energy optimisation

For a long time, k_La-based models have been used to capture mass transfer between the gas and adjacent phases during aeration. More recently, models taking air flow rate as input were proposed. Despite the inclusion of somewhat more complexity and the resulting improved model performance, the variability of the α "fudging factor" in space could still not be entirely related to process variables such as sludge concentration and sludge age, i.e. a lot of unexplained variance remains. Moreover, α was shown to vary spatially in a reactor (Rosso et al., 2011). This spatial variation introduces a significant amount of uncertainty in the model prediction when a single α value is used, resulting in locally different dissolved oxygen concentrations and, hence, aerobic process rates.

To date, a key assumption in all aeration models is assigning a single average bubble size. This assumption is not very apparent, but resides in the gas-liquid interface surface area (a) of K_La and is hidden in the α value in oxygen transfer efficiency (OTE) based models. This constant bubble size assumption is unrealistic and can be very restrictive for the model since the bubble's interfacial area drives the oxygen transfer process. In reality, bubble size is spatially distributed (Fig. 3, left) from the point of injection to the top of a reactor due to the process of coalescence leading to a significantly different bubble size distribution near the reactor top. Another factor that plays a role here is the fact that there are pressure differences

when moving from the bottom to the top of the reactor, and these will also influence bubble size. Increased viscosity (due to the presence of sludge) further promotes coalescence compared to clean water (Fig. 4) (Fabiyi and Novak, 2008; Ratkovich et al., 2013). A PBM using bubble size as the internal coordinate and including coalescence as a PBM reaction process can significantly improve the local prediction of oxygen mass transfer (and hence α) as well as improve the design of aeration systems to maximize the oxygen transfer (in combination with Computational Fluid Dynamics - CFD). It should be noted that the current work in CFD linked to aeration also uses a fixed bubble size (Fayolle et al., 2007). The use of PBMs in aeration systems with suspended solids has not been widely studied in WWT. PBMs applied to bubble columns are widespread in fermentation systems and the chemical engineering literature (Wang, 2011; Dhanasekharan et al., 2005; Sanyal et al., 2005) and can serve as a solid examples of improved benefits to these process models.
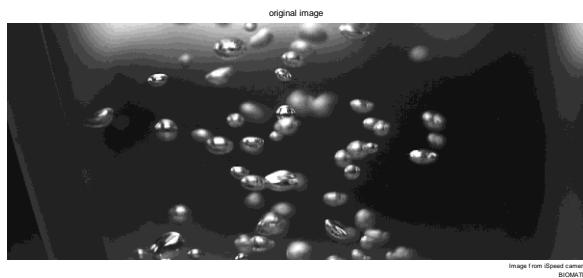

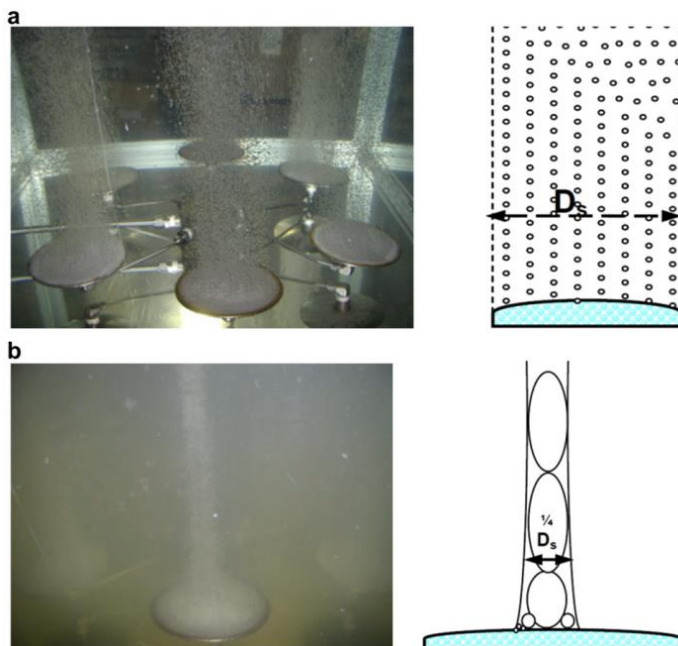Fig. 3 – Illustration of variability in bubble size as measured with a high speed camera

Fig.4 - Impact of viscosity on bubble coalescence

Typical mechanisms taking place in bubble breakup and coalescence are shown in Fig. 5. The kernels used in a PBM describing bubble breakup and coalescence are very similar as those used in a flocculation PBM.
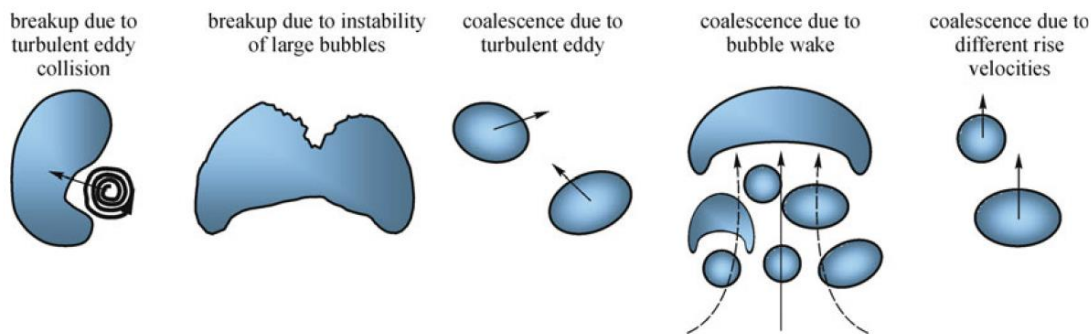
Fig. 5 - Bubble breakup and coalescence due to different mechanisms (after Wang, 2011).

Floc and granule size: distributed kinetics

Despite the fact that the size of agglomerates, be it flocs or granules, can play an important role in biological activity (e.g. different microbial consortia at different locations in the agglomerate), the simulation of such a microenvironment within a macro-scale fluid transport environment has hardly been performed. Recently, Volcke et al. (2012) demonstrated the significant impact of granule size distribution on the performance of an Anammox-based granular sludge reactor. The authors used a fixed size distribution for this analysis. It is clear that size distribution can be impacted by shear and, hence, will further influence the system behaviour. The absence of size and size dynamics in the currently used models indicates that the activity loss caused by particle size (causing transport limitation due to stratification, e.g. Vangsgaard et al., 2012) cannot be predicted by current models. Again, when experimental data are confronted with these models, other degrees of freedom (i.e. parameters or input variables) will be calibrated for inappropriate reasons.

Sobremisana et al. (2011) demonstrated that including floc size can result in significantly deviating reactor performance since kinetics can be quite different depending on reactor location and the size of the biological floc. The authors used an integrated PBM-CFD approach to simulate the carbon and nitrogen removal process at both the reactor scale and internal floc scale. The effect of size was introduced by means of an effectiveness factor (i.e. ratio of rate with and without diffusional resistance) based on floc size for all different processes. For a simple baffled reactor the treatment performance deviated by 13% for COD, 10% for NH_4 and 56% for NO_3 compared to the same simulation not accounting for influence of size. However, further validation is required.

Knowledge arising from this can be useful to (partially) decouple affinity constants in kinetic rate expressions and reduce their requirement for calibration. Understanding the interaction between size and reaction kinetics can inform researchers and engineers on how to better design and operate these processes (e.g. avoid or promote certain shear zones and account for imposed shear of mixing and aeration intensities). Moreover, it will reduce the need to adjust parameters unnecessarily to improve the model fit.

Apart from size heterogeneity, incomplete mixing can lead to spatial heterogeneous concentrations in biomass and substrates that ultimately result in locally different kinetics. Integrating the effects of spatial variations in macroscale mixing as well as the biomass and substrate concentration is another avenue for further model development. Lencastre Fernandes et al. (2013) demonstrated the effect of this heterogeneity for a budding yeast population using a multi-scale modelling approach that included PBM. A similar approach could be used for WWT modelling, and could be helpful in developing an improved understanding of

biomass population dynamics. A complicating factor for the WWT compared to a yeast fermentation is that multiple species have to be considered to model the WWT appropriately.

Models including floc size and local heterogeneities could also be helpful in developing technologies to select between wanted and unwanted microbial communities, which is a recently developing topic in view of mainstream Anammox application. Microbial selection can be done on a physical basis (size) or through selection by creating favourable growth conditions for the targeted microbial consortium (Al-Omari et al., 2014).

Precipitation/crystallisation for better quality marketable products
WWTPs are transforming into WRRFs (Water Resource Recovery Facilities) leading to new modelling challenges (Vanrolleghem, 2013). One important aspect in product recovery, driving their market value, will be the specifications of the recovered material. These comprise both composition and size. Crystallisation has been extensively modelled in the field of chemical engineering and pharmaceutical engineering to produce crystals with tailor-made specs (e.g. Aamir et al., 2009, Nagy and Braatz, 2012). A PBM with crystal size as an internal coordinate and inclusion of nucleation (function of supersaturation) and crystal growth can be used as a first approximation. If needed, more internal coordinates can be added to deal with composition or crystal shape (e.g. 2-D compared to 1-D, Samad et al., 2011). Additional phenomena such as agglomeration and breakage can be added. Interestingly, describing crystallisation with a PBM also allows describing phenomena such as size-dependent crystal growth (Samad et al., 2011).
The use of a PBM modelling framework is widely accepted when studying crystallization processes. However, in a WRRF context the PBM framework has not really been used thus far, with the exception of a recent manuscript by Galbraith and Schneider (2014) where a discretized PBM was used to describe the chemical precipitation of phosphorus. The most important discussion points, when implementing a PBM, are usually related to the model assumptions (which phenomena should be included?), and to the selection of the kinetic expressions for each phenomenon that is included in the PBM. The main phenomena are nucleation, crystal growth and dissolution (= negative growth), agglomeration and breakage. However, it happens frequently that the PBM only considers growth and nucleation (Fujiwara et al., 2005). Another important variable that needs to be included in these models is the super-saturation, which will vary as a function of temperature and is usually represented as a polynomial describing the super-saturation curve as a function of temperature.

CONCLUSIONS
Many processes in WWTPs are governed by population dynamics of materials characterised by variation in property dynamics. These potential complexities in system behaviour are lost or significantly suppressed when only average behaviour is characterized or simulated. Population Balance Models can deal with these process complexities and have already demonstrated their benefits in the field of (bio)chemical engineering. The majority of the models in WWT modelling that need more rigour are physical-chemical processes. Hence, more than ever we need to look over the fence and integrate available (bio)chemical engineering knowledge into WWTP models. Some examples are described in this paper, but potentially many more applications of PBM in WWT exist and can be exploited. The intention of this paper is to make WWT modellers aware of this framework and its potential applications, challenges, and pitfalls.

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