Multi-Scale Additive Manufacturing Lab (MSAM)
Mechanical and Mechatronics Engineering
University of Waterloo

AM Pure

The Antimicrobial Water Bottle

Project team

B.Sc. Kai-Uwe Beuerlein
Graduate Student
kai-uwe.beuerlein@uwaterloo.ca

M.Sc. Cara Greta Kolb
Graduate Student
cgkolb@uwaterloo.ca

Prof. Saeed Maleksaeedi
Assistant Professor
saeed.maleksaeedi@uwaterloo.ca

Abstract

The availability of safe drinking water is a fundamental need for human beings. Environmental conditions and low waste management standards jeopardize the quality of this important commodity in large areas of the worlds. Particularly affected are electricity-poor regions, which only have limited access to advanced water purification methods (HORVÁTH et al. 2022). Photocatalytic water treatment which uses sunlight to chemically activate titanium dioxide (TiO_2) represents a promising approach to face these precarious circumstances (MCCULLAGH et al. 2007; REDDY et al. 2017).
AM Pure is an additively manufactured water bottle that uses this mechanism to provide safe and clean hydration on-the-go. The bottle features a novel design that leverages gyroid structures to act as fibre optics. Light rays are efficiently captured by the unique surface texture and transported to the inside through a network of gyroid structures. A special design of the core and the shell of the gyroid structures leads to a targeted homogeneous exit of the light rays over the entire enormous surface area. The ultraviolet component of the light rays is the initial trigger for the chain reactions to kill the pathogenic species present in the surrounding water. Simultaneously, **AM Pure** allows to easily separate sediments that collect at the bottom. Tesla valves prevent the particles from flowing back when drinking.
Consequently, **AM Pure** is a bottle that not only provides pure and hygienic water every time you take a sip, but also looks sleek and stylish. Say goodbye to germs and hello to clean water.

Contents

Chapter 1

Industry Overview

The universal access to clean drinking water in sufficient quantities is vital for human life. Economic growth and technological progress have led to significant improvements in the water quality in recent decades. However, even nowadays, people in large parts of the world still do no have access to safe drinking water owing to various contamination risks and insufficient sanitary conditions. Around the globe, at least 1.8 billion people drink water that is polluted by feces (BAIN et al. 2014; WHO 2017). According to the World Health Organization (WHO), the global disbursements for humanitarian aid spent on water and sanitation were 6.9 billion USD in 2015 and 2017 (WHO 2019). The United Nations Children's Fund (UNICEF) alone procured 154.4 million USD in 2021 (UNICEF 2023).

The shortage in clean drinking water is particularly acute in areas which are affected by natural or man-made disasters. Projections even anticipate that the frequency, intensity, and duration of natural catastrophes are likely to increase significantly due to the deteriorating climate change (BANHOLZER et al. 2014; SAUERBORN and EBI 2012). Those events are likely to cause the sanitary infrastructure to be disrupted (HORVÁTH et al. 2022). This is usually accompanied by a breakdown of the power supply, which impedes the application of electricity-driven methods to purify water (RAY and JAIN 2014). Under such circumstances, the affected population is forced to drink water, which may be severely contaminated (HORVÁTH et al. 2022). Particular hazards arise from feces and parasites as well as life-threatening bacteria and viruses (PAL et al. 2018). This elucidates the necessity to identify efficient methods to purify water that do not require a power supply.

Chapter 2

Design, Functionality and Durability

AM Pure presents a unique design to simultaneously decontaminate water and remove sediments. Gyroid structures as well as a tesla valves are leveraged to achieve this aim (see Figure 2.1). For a detailed description of the geometry, including dimensions and tolerances, the reader is referred to the appendix (see Figure A.1).

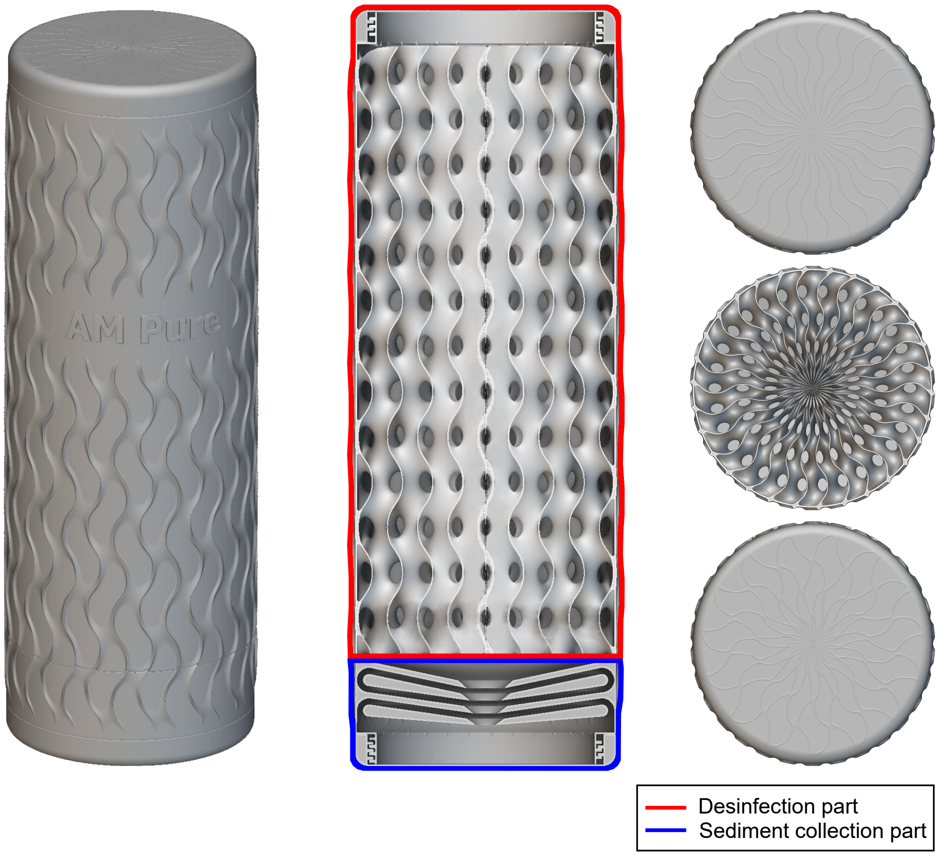

Figure 2.1: Design of **AM Pure**

The unique operating principle of **AM Pure** is founded on three main mechanisms. These encompass the efficient capture of light rays and their transmission to the inside, the targeted photocatalytic reaction with TiO_2, and the separation and collection of sediments. The respective processes are further outlined below.

Efficient capture of light rays and transmission to the inside

The external surfaces of **AM Pure** are characterized by gyroid textures that allow the light rays to enter the *shell optics*. Shell optics enable light rays to be transmitted through their body, but unlike conventional fiber optics, they do not have a circular cross-section. The capture of light is further facilitated by the convex curvature, which acts like a converging lens. Light rays that do not reach the gyroid texture, transmit through the unstructured shell surface and readily react with the present TiO_2. The transmission in the shell optics relies on total internal reflection. Minor differences in the refractive index between the core and the shell of the shell optics cause the light rays to be deflected (see Figure 2.2). Using a graded transition of the refractive index across the width of the shell optics results in sinusoidal deflections of the light rays.

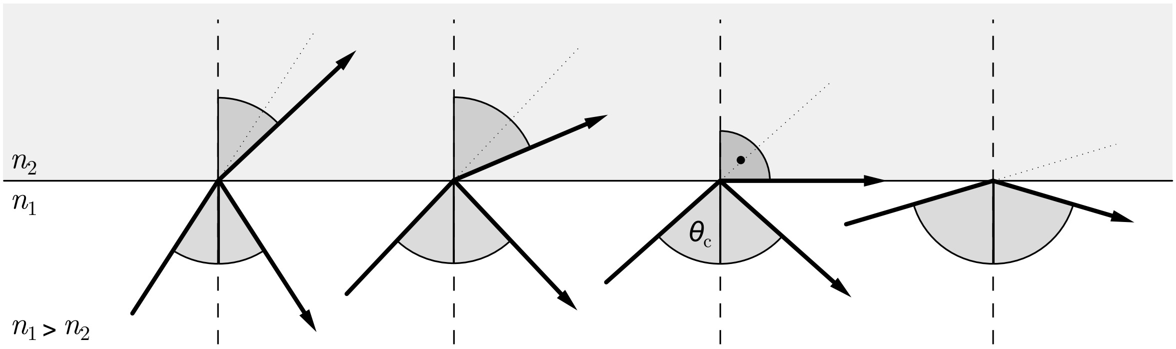

Figure 2.2: Refraction of light for several angles of incidence at different refractive indices n_1 and n_2; appearance of total internal reflection above the critical angle θ_c.

The critical angle θ_c for total internal reflection is given by the Snell's law:

$$\theta_c = \arcsin\left(\frac{n_2}{n_1}\right), \tag{2.1}$$

with the refractive indices of the two materials n_1 and n_2.

If the angle of incidence is higher than θ_c, the light ray is entirely reflected on the inner surface of the shell. A targeted adaptation of the refractive index is conceivable by incorporating nanoparticles into the raw material or adjusting the process parameters to vary the degree of curing.

Overall, this effects a targeted migration of ultraviolet light deep into **AM Pure**. Intentionally introduced defects and manufacturing inaccuracies, such as due to the staircase effect, cause part of the light rays to leave the shell along the way and to initiate the reaction with TiO_2 (see Figure 2.3). This is even enhanced by a targeted decrease of the angle of curvature towards the center. Accordingly, the intensity of radiation is constant at a lower mean nominal light intensity in the shell optic.

Photocatalytic reation of TiO_2

The photocatalytic reaction is based on the chemical activation of titanium dioxide TiO_2 by ultraviolet radiation (McCullagh et al. 2007; Reddy et al. 2017). This approach of purifying water has been researched for over several decades and its feasibility demonstrated in various publications (Matsunaga et al. 1985; Matthews 1987).

TiO_2 exhibits the ability to efficiently absorb the ultraviolet fraction of the sunlight spectrum (McCullagh et al. 2007; Reddy et al. 2017). When in contact with water, this initiates a series of reactions, which lead to the formation of highly reactive oxygen species (ROS) (Reddy et al. 2017):

$$H_2O + h\nu \xrightarrow{TiO_2} ROS$$

Before decaying, the ROS can attack the water contaminants in the immediate vicinity of the surface and make them harmless to humans. The superior specific surface area of the gyroid structures thus leverages the efficient decontamination of the total water contained in the respective chambers (see also Figure 2.3).

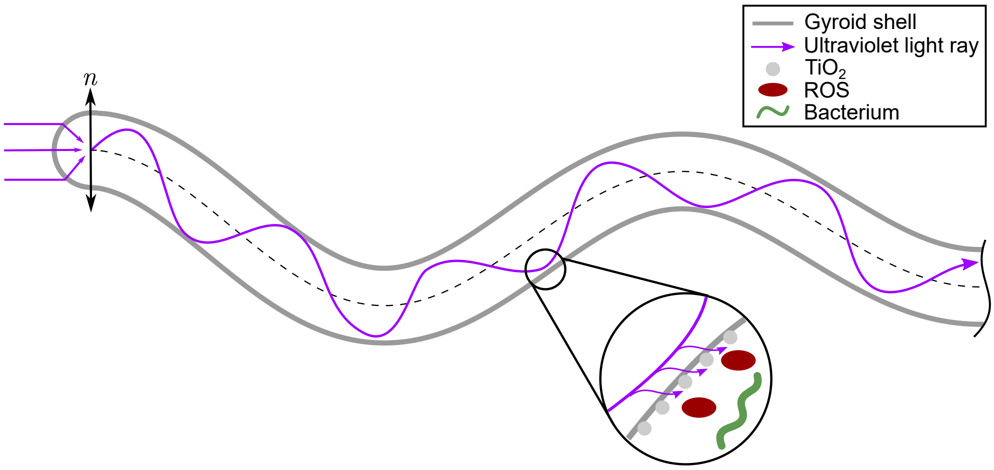

Figure 2.3: Functional principle of **AM Pure**: Captured ultraviolet light rays are transmitted via total interal reflection caused by the graded refraction index n along the gyroid structure; rays leaving the gyroid interact with the TiO_2 to form ROS.

Separation and collection of sediments

Contaminations due to particles can be of miscellaneous nature, such as sand and rust (COLTER and MAHLER 2006; GUCHI 2015). The diameter of these particles is usually in the magnitude of several 100 µm to a few mm. According to the Péclet number, which is based on the Stokes' law, the particle movement is thus governed by gravity rather than Brownian molecular motion (MEWIS 1996; RAMASWAMY 2001). This forces the particles to settle to the bottom of **AM Pure**. The mechanism strongly depends on the particle diameter, such that larger particles settle faster (MEWIS 1996).

Aiming at collecting and separating the sediments at the bottom, a unique design is incorporated in the main body of **AM Pure**. This consists of two units acting as tesla valves with an attached collection container (TESLA 1920). These structures exhibit a lower flow resistance in one flow direction than in the reverse flow direction. This allows the sediments to settle in the collection container, but prevents them from travelling back while drinking (see Figure 2.4). The collection container can be removed from the main body for cleaning.

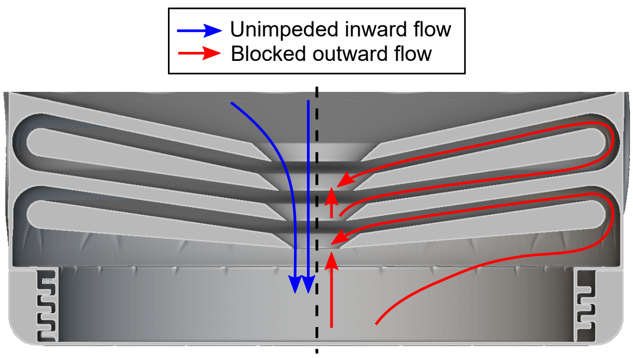

Figure 2.4: Functionality of the tesla valve; left: unimpeded inward flow enables the sedimentation of particles; right: blocked outward flow prevents particles from leaving the container when drinking; attachment of the inner structures to the outer wall outside the section plane.

Chapter 3

Design Integration and Utilization of DDM Materials and Processes

Digital process chain
AM Pure relies on an end-to-end digital data chain, which allows to thoroughly plan and prepare the subsequent building job. The digital design is achieved through sophisticated computer-aided design programs, such as *nTopology*, which enable novel geometries based on numerical calculations. Hence, the existing design features are no longer defined by only geometrical dependencies, but mathematical surface optimizations. This leads to the generation of gyroid structures, which represent the mathematically optimized shape at maximum surface-area-to-volume ratio. In this context, the angle of incidence can be predicted at any point of the external gyroid textures. This allows to adjust the geometry a priori and thus to ensure that the angle does not deceed the critical angle for total internal reflection. Cylindrical cell maps are used to determine the required angles of curvature as a function of the distance to the center. The automated control of the individual print nozzles enables the selective introduction of nanoparticles into the base material. This voxel-based manufacturing approach can only be realized by digitalized preprocessing and additive manufacturing processes. The design phase is followed by the remaining state-of-the-art process steps of the build job preparation. Due to the self-supporting property of the gyroid structures, AM Pure requires very little support material. The support structure that is required in few places is created automatically during the build job preparation. By using soluble material for this, it can be easily removed in a post-process.

Technologies and materials
The technologies pertaining to the *Material Jetting* category according to ISO/ASTM 52900 are predestined to realize **AM Pure**. Particular suitability is expected by the MultiJet Modeling (MJM) process, in which a liquid photopolymer is deposited drop by drop onto a substrate. Due to the intentionally set overlap, the drops merge into a homogeneous layer structure. The technology merits specific attention for **AM Pure** due to its superior printing resolution, the excellent multi-material capability, and scalability. Beside *Material Jetting*, a realization of **AM Pure** through a *Material Extrusion* process, such as Direct Ink Writing (DIW) or *Binder Jetting* (BJ) also appears to be feasible. The proposed processes, in particular MJM and BJ, also allow for a voxel-precise material design. Accordingly, every single voxel is intentionally assigned to a specific base material. This also facilitates graded structures, which are expected to result in areas of different refractive indices, as required for **AM Pure**.
Due to the unique function principle, **AM Pure** requires a transparent biocompatible resin. This applies for the custom material *VeroClear*, which is intended to imitate poly(methyl methacrylate) (PMMA). In addition, cheaper materials, such as PMMA itself or polycarbonates (PC), are also conceivable, if they are qualified for the selected process.

The TiO_2 particles can be homogeneously deposited onto the gyroid shell surfaces by several chemical or physical processes upon the build job, such as chemical vapor deposition (CVP) or physical vapor deposition (PVD) techniques. Aiming at an end-to-end process without any post-processing steps, the TiO_2 can be also incorporated into a solvent to prepare a printable ink and deposited in-situ.

Chapter 4

Digital and Physical Infrastructure: Systems Integration, Utilization, Value Chain Leverage, Agility, Lean and Continuous Improvement

Currently, the use of digital designs to support humanitarian aid plays a minor role in crisis management. Governments and private individuals predominantly provide financial support and aid supplies, which often requires transports over thousands of kilometers to remote locations. This often leads to distinct delays in the arrival of urgently needed goods. Additive manufacturing promises to contribute to rapid crisis management. Engineers around the globe can be mobilized to virtually develop individual solutions. This could also revolutionize charity work, as individuals are asked to donate time to create digital designs. Through the virtual exchange of the relevant design data, decentralized manufacturing allows to directly fabricate the parts in the affected areas without the necessity of various raw materials and pre-products (BEN-NER and SIEMSEN 2017). Unlike in traditional manufacturing processes, these technologies do not require the utilization of tools and dies (GIBSON et al. 2015). In addition, the predominantly digital and lean process chain allows the product design to be quickly and efficiently adapted to changing conditions, making it robust even in crisis areas.

Chapter 5

Cost Benefit/Value Analysis

Safe drinking water is an essential element for human life and thus its accessibility is considered a fundamental human right. While it is possible to assign a monetary value to water based on the cost of infrastructure, treatment, and distribution, its inherent value cannot be priced. **AM Pure** contributes to this overall aim by providing clean water at low costs. The total costs per part are estimated to 64.12 $ (see Table 5.1). This refers to the fabrication via the MJM process and the use of the transparent material *VeroClear*. Additional costs that are difficult to evaluate, such as costs for nanoparticles and support structures, were combined into an added overhead factor of 30%. Employing less cost-effective materials (see Chapter 3) can significantly reduce the total costs (CHEN et al. 2021). During lifetime, no additional costs emerge due to e.g. maintenance or operating costs.

As the MJM process and related technologies exhibit a high technology readiness level and strongly rely on the digital preparation without extensive physical pre-processing, a subsequent evaluation of the part quality is not considered to be required. The high resolution of the MJM process is inherent to its nature and the evolution from the conventional two-dimensional printing process. Therefore, the tolerances provided (see Figure A.1) already allow manufacturing with a fast mode of the machine. Further relaxation of the tolerances does not offer any additional opportunity for cost savings.

These advancements in technology can help to make safe drinking water accessible and affordable to more people, especially in crisis-affected regions where cost is a major concern.

Table 5.1: Estimation of the total costs per part

Total material costs per part	**55.68 $**
Part mass	0.184 kg
Material costs	302.5 $ kg^{-1}
Total machine costs per part	**8.44 $**
Machine purchase costs	300,000 $
Machine lifetime	10 years
Machine utilization	90%
Part volume	$102.3\,\mathrm{cm}^3$
Build rate	$1.16\,\mathrm{cm}^3\,\mathrm{min}^{-1}$
Parts per build volume	16
Build time per part	88.2 min
Overhead	30%
Total costs per part	**64.12 $**

Chapter 6

Conclusions

AM Pure is an additively manufactured water bottle, that facilitates the decontamination of water from pathogenic species and sediments without electrical power. The purification is based on two key mechanisms. Pathogenic species are killed through the reactants resulting from the photocatalysis of $\mathrm{TiO_2}$ with ultraviolet light. Owing to its unique geometry based on a network of gyroid structures, **AM Pure** effectively captures sunlight on the outer bottle shell and transports it to the inside. A novel design of the core and the shell of the gyroid structures allows for a targeted homogeneous exit of the light rays over the entire superior surface area and a rapid reaction with the $\mathrm{TiO_2}$ incorporated in the shell. The sediments are collected at the bottom of **AM Pure**, whereby tesla valves prevent the backflow of the particles.

Due to its sophisticated design, **AM Pure** can only be realized through additive manufacturing. Its inherent characteristics make **AM Pure** predestined for the MJM process, although also the application of related liquid-based technologies and BJ is conceivable. These mature processes with a high reproducibility achieve the required high resolutions and facilitate the multi-material processability of different raw material compositions. A digital process chain was set up, which incorporates all required steps to thoroughly plan, predict and adjust the design virtually and also accounts for the voxel-based material allocation.

Due to the ubiquitous need for safe water and thus the enormous global efforts especially in crisis areas and underdeveloped countries, **AM Pure** has a great potential to broadly improve the living conditions. The key operating principle of **AM Pure** is expected to be easily scalable to larger dimensions and customized to related applications. This opens up tremendous new application fields, such as the implementation of the key principle in water tanks.

Appendix A

Technical Drawing

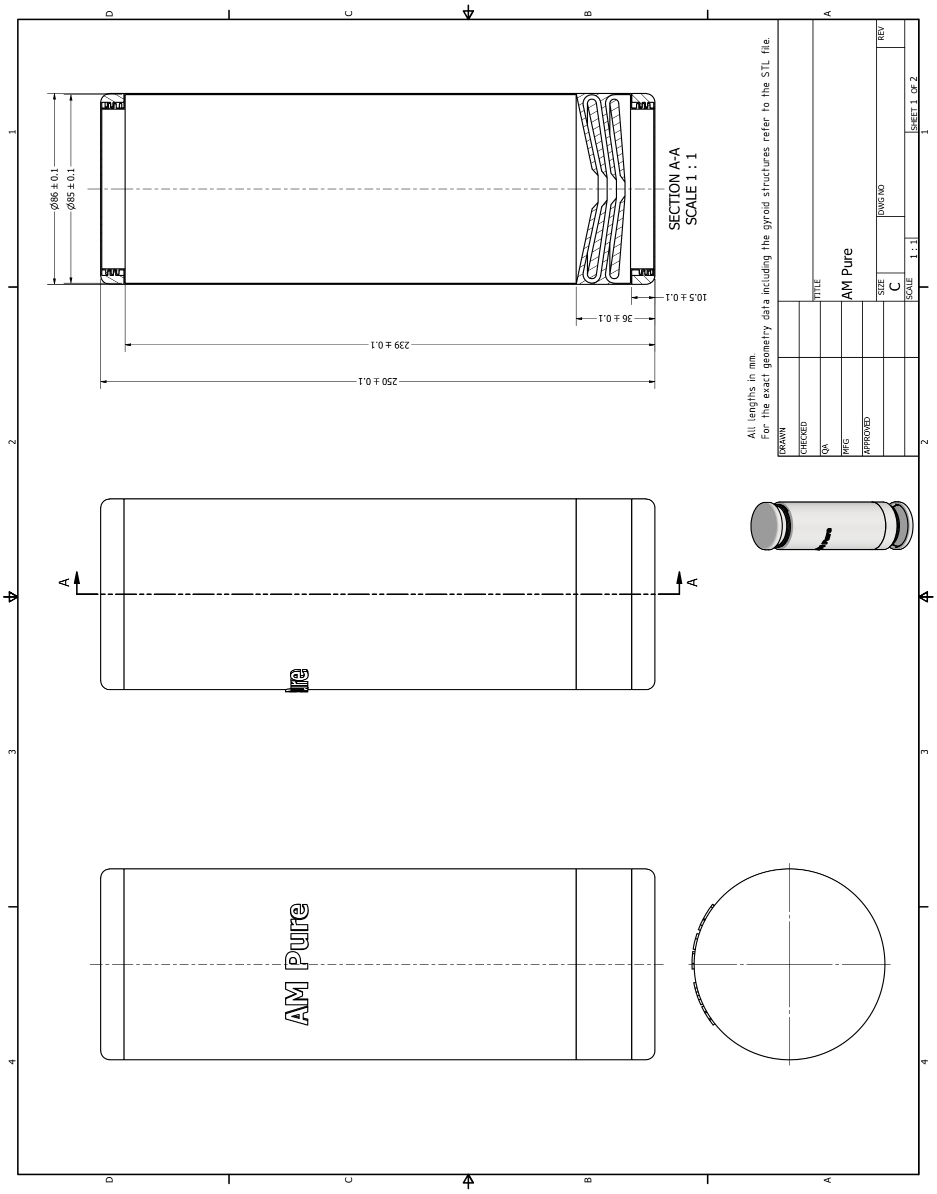

Figure A.1: Three view drawing of **AM Pure** with dimensions and tolerances; for the exact geometry data including the gyroid structures refer to the STL file.

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