State of the art of UV water treatment technologies and hydraulic design optimisation using computational modelling

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Highlights

- Effectiveness of UV in comparison with other water disinfection technologies
- Beneficial use of CFD in optimisaton of the Geometrical features of UV technology
- Investigating the effect of Geometry on the UV dose received by the water
- Exploration of various turbulence and fluence modelling affecting UV technology
- Scope and appraisal of using LED lamps in full-scale water treatment plants

Abstract:

Water disinfection is an essential process for drinking water use. One of the water treatment process stages includes the application of Ultraviolet (UV) light to assist with the removal of pathogens and viruses such as Cryptosporidium. The previous review in the UV treatment system explores the optical and reaction of microorganisms to the technology. The aim of this paper is to explore the hydraulics and modelling of the current technology of the UV treatment process. There has been enormous progress made in the process of optimisation using Computational Fluid Dynamics (CFD). Due to the expensive nature of the experiments, CFD has emerged as a vital tool. This article explores two essential parts of the UV system that includes the hydraulic system and the modelling. It also explores the effects of design improvements on the UV dosage and overall disinfection efficiency.

1.Introduction

The two primary sources of potable water available for community use include surface water and groundwater. Surface water contamination includes viruses, bacteria, and protozoa [1]. Thus, the use of surface water for drinking purposes requires treatment through various disinfection processes that involve the use of free Chlorine, Chloramine, Chlorine dioxide, Ozone and Ultraviolet Light (UV). Each of these processes is chemical processes except for the use of UV. Currently, water companies use primarily chlorinate ion for the treatment of water. However, chlorination and UV treatment have an inverse relationship in treating different types of pathogens [2]. Pathogens such as Cryptosporidium and Giardia lamblia cysts display a higher level of sensitivity to UV and are quite insensitive to the chlorination process [3]. Ozone treatment is another process that is more effective than chlorination in treating such pathogens. However, it has disadvantages, including the creation of chemicals on-site and by-products from the treatment process[1,4,5].

Table 1: Effectiveness of disinfection processes against pathogens

Types of pollutants	Free chlorine	Chloramine	Chlorine dioxide	Ozone	UV
Bacteria	Excellent	Good	Excellent	Excellent	Good
Viruses	Excellent	Fair	Excellent	Excellent	Fair
Protozoa	Fair to poor	poor	Good	Good	Excellent

Table 1 indicates that different pollutants possess a varying sensitivity in relation to the disinfection process [1]. Therefore, a process that includes a combination of the required properties will produce the best results for the overall water disinfection effectiveness. Using multiple disinfectants will also lead to the lower usage of chlorine, thus producing a reduced amount of chlorine by-products in the water. Figure 1 below indicates that in order to accomplish a 4-log inactivation of different pathogens, there is a varying level of dosage required in terms of UV and Chlorine. The product of intensity and irradiance time defines the UV dosage value. Combining the product of intensity and irradiance time it reduces the amount of dosage required from chlorination and UV. Increasing the UV dosage does not produce any adverse effects because there are no by-products created, although producing a higher UV dosage is expensive [2]. In addition, the combination of UV and Chlorine requires a substantially reduced amount of chlorination, which in turn produces an even smaller quantity of by-product compounds like Trihalomethanes (TTHMs). Figure 1clearly indicates the regulatory limits for the presence of these compounds in potable water. The use of UV offers several other advantages compared to the chemical processes, including the facts that it can be used instantaneously without having the requirement to handle chemicals [2,4].

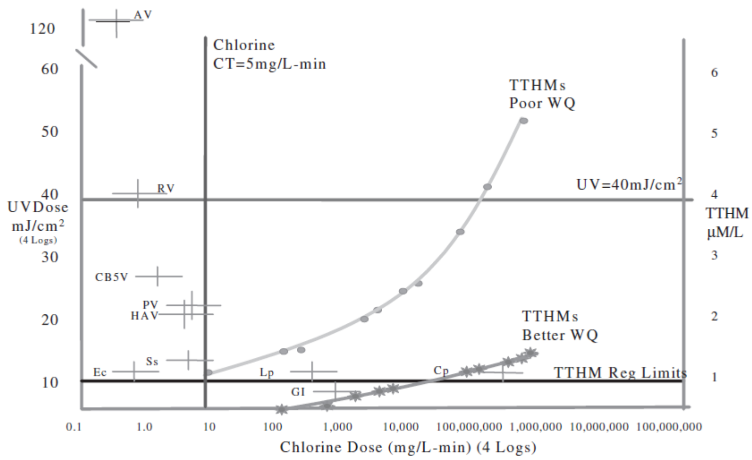

Figure 1: Chlorine dose vs UV dose vs TTHM for 4 log reduction of pathogens [2]

1.1 Current UV treatment systems

The current UV treatment process predominantly uses low or medium pressure mercury lamps to produce UV light [6]. The medium pressure mercury lamps produce polychromatic light, i.e. light in the range of 200-400 nm, while the low-pressure mercury lamps produce monochromatic light and emit at 253.7nm. UV light-emitting at 260-265nm disturbs the DNA of most pathogens. Thus, low-pressure lamps are more efficient compared to medium pressure mercury lamps [7]. The effect of UV dosages is a measure of the effectiveness of UV treatment. The product of intensity and irradiance time defines the UV dosage value [2]. The ideal system requires a uniform dosage distribution inside the water reactor.

The classification of UV disinfection reactors includes three types of reactor, external, distributive and immersive type. The external type UV reactor has the UV lamps placed outside of the water flow and light transmitted through the Quartz pipe. The distributive type of reactor UV has rays transmitted to the water body using a medium like a glass rod or optical fibre. The most common and widely used in the industry is the immersive type of reactor. This type of reactor has lamps placed inside the reactor and the flow of water around the lamps. The lamps placed perpendicular or parallel to the water flow, depending on the arrangement type. Similarly, based on the UV lamps' location, the classification includes two different types the contact and the non-contact type. Currently, the most used contact type of reactors has mercury UV lamps inside the water reactor. This is like the immersive type of water reactor [8]. Table 2 is used to summarise the type of UV source used for the UV disinfection technology.

The validation of the UV treatment system is done using Bioassay protocol. In this test, MS2 is introduced in the upstream of the flow and passed through UV reactor chamber. The sample is then collected downstream of the flow. The difference in the quality of the water is analysed in terms of log reduction. It requires 4 log inactivation (99.99%) of pathogens and virus for drinking water application. Two different ways of measuring UV dosage is by calculating the average dosage and Reduction Equivalent Dose (RED). The average dosage could give false information since some pathogen might be receiving a very high dosage while some pathogens are receiving low dosage. This can be overcome by calculating RED values, which calculate the minimum dose received by the pathogen. Research has been done in alternative validation methods such as using monitored tunable biodosimetry (MTB) and using photochromic materials. However, the current commercial UV treatment system is validated using biodosimetry [2, 9-11].

Table 2: Type of UV sources

Type of UV source	References
Mercury - low pressure lamps	[8–31]
Mercury - medium pressure lamps	[32–37]
LED lamps	[6,7,38–59]
Source not mentioned	[2,60–72]

2. Modelling of UV treatment System

The UV modelling includes two sections: 1) modelling of the flow inside the reactor and 2) Modelling of the UV fluence rate inside the reactor. The two different methodologies usually adopted for modelling include SURF (Simultaneous UV fluence rate and Fluid dynamics) and TURF (Three-step UV fluence rate and Fluid dynamics). The SURF method incorporates simultaneous UV fluence rate and Fluid dynamics. This method defines the UV fluence rate using a user-defined function in the CFD software. In comparison, the TURF method includes a three-step UV fluence rate and Fluid dynamics. This method carries out separate calculations for the UV fluence rate and the flow calculation [62,73]. In addition, another method used, carries out the simultaneous calculation of the UV fluence rate along with the flow calculations using UDF (user-defined function). However, post-processing is carried out separately using a specific written code [17].

2.1Modelling of flow (CFD)

2.1.1Mesh

Mesh independency tests are carried out for the simulations. The mesh size can vary due to several factors, including different sizes and other characteristics of the reactor. For some models, 0.5 million cells are adequate, while others require more than 2 million cells [17,62,69,73]. However, in these models, increasing the number of cells, the deviation of the result is less than 2%. Thus, the mesh considered acceptable for the result.

The mesh independency test carried out uses the residence time distribution of the particle paths. Thus, convergence achieved at 5000 particles. Increasing the particles number does not alter the residence time [22,31,74].

Across the flow, micro particles released at the inlet assist with understanding the flow pattern of microorganisms in the water. The number of microbial particles released varies for different reactors and simulations. In addition, the microbial particles size also varies. Particles assist the calculation of the microbes' flow trajectories inside the reactor. The particles size is as small as 10^{-6} m in diameter. It is important to understand that the diameter should not affect the result of the simulation [2,10,15,17,18,21,22,31,36,37,62,66,69,71,73,74].

2.1.2 Model settings

Model settings are dependent on the reactor type being a closed conduit or an open channel reactor. Open channel reactors are more demanding to model as they incorporate both air and water. The flow temperature considered as constant [20].

2.1.3 Boundary settings

The flow velocity and reactor conditions form the basis for the inlet and outlet conditions. Usually, the inlet is applied using flow velocity perpendicular to the inlet surface. The specified inlet turbulence intensity is 2% to 3%. The turbulent intensity at the inlet has little effect on the simulation. The outlet conditions taken as outlet pressure, set to 0-bar gauge pressure. The walls are set as no-slip boundary conditions [17,69].

2.1.4 Turbulence model

Different turbulence models such as standard k-ε, realisable k-ε, k-ω, Reynold stress model and two fluid model compared for closed conduit water flow. It is worth noticing that the k-ε model can better predict the wake-free model than the k-ω model. Thus, it predicts the upstream flow pattern more accurately using k-ε rather than a k-ω model. However, the much more precise wake region prediction uses the k-ω model. Additionally, it is also worth noting that the RSTM predicted model performs better than the k-ε model both inside and outside the wake region. However, it is not able to predict the wake region as accurately as the k-ω model. The judgement for this comparison uses the experimental data from a PIV experiment. Because of the different flow pattern, there is a turbulence model effect on the UV dose distribution. The difference highlighted in terms of the dominant peak and secondary peak of the dose distribution. There is both dominant and secondary peak in std k-ε, realisable k-ε, k-ω, RNG and TFM. In the RTSM model, there is no secondary peak, because of better flow near the wall region. k-ω has neither a dominant nor a secondary peak and observes a wider spread of the UV dose distribution. The Reynold stress model provides similar results for velocity and dosages but more significant variation in the turbulent kinetic energy [75]. Additionally, comparison carried out for the k-ε model, RNG k-ε model and Reynold stress model. The k-ε model considered adequate, as there is a slight difference in the value of velocity and dosages. The k-ε model is 3-4 times cheaper compared to the Reynold stress model [25]. However, k-ε model fails to accurately predict the disinfection model for certain geometry such as introduction of baffle upstream of the flow. Higher turbulence model such as LES are required to correctly calculate the wakes created because of the obstruction in the flow [60]. There is an effect on the mass transfer rate because of the flow in certain UV processes like Advanced Oxidation Process (AOP). However, those effects are not studied for the UV treatment of drinking water application [61].

2.2 UV modelling (UV Fluence)

The UV modelling helps to determine the fluence rate inside the reactor. The UV modelling carried out either through user-defined function in CFD or through separate modelling using software like MATLAB. There are different type of models used for modelling the fluence distribution inside the reactor. Most commonly used models are MPSS and MSSS models.

MPSS (Multi point source summation model) model

The MPSS model used to simulate the fluence rate field inside the reactor. The MPSS model considers each lamp as a collection of light-emitting point sources of equal power. Considers the light emitted is in an axial direction. Each point receives a fluence rate equalling to the total fluence rate received from each point source. The calculated light beam laws use Snell's law and Fresnel's law. The calculation for the absorption law uses the Beer-Lambert's law [62,73].

MSSS (Multi segment source summation model)

The MSSS model is like the MPSS model in terms of refraction reflection and adsorption; however, it considers the lamp as a cylindrical source. The light intensity decreases with the cosine angle between the unit normal vector and the directional vector. The MSSS model is computationally expensive compared to other models [62,73]. Table 3 summarises the type of modelling software used to calculate the dosage data for the UV treatment system and the fluid data such as the turbulence model used.

Table 3: Fluid flow vs Turbulence model vs UV fluence modelling

Fluid flow modelling software	Turbulence model	UV Fluence modelling	References
Ansys Fluent	k-ε	Calc3D	[34,36]
		Integrated model in fluent	[18,19,33,64,65,69,71]
		User defined functions in fluent	[8,17,22,66]
		MATLAB	[62,73]
Ansys CFX	k-ω SST	Calc3D	[31]
COMSOL	k-ε	Not mentioned	[60,61,74]
	Large eddy simulation (LES)		[60]
	Not given		[7,41,48]
COMET	k-ε		[68]
PHOENICS			[27,29,75]
Finlab			[5]
Not required		MATLAB	[10–12,44,54,70]
Not mentioned		Not mentioned	[30,32,76,77]

3. Hydraulic Systems

The current reactor geometry's main division includes two-sub sections, the open channel and the closed channel, reactor [37]. The closed reactors' primary use is for drinking water applications, while the open channel reactors are commonly used for wastewater applications.

However, there has been research carried out for open channel drinking water applications. The advantages of an open channel reactor to the closed reactor include the flow that can be highly turbulent, and therefore cheaper to install. Similarly, there has been research carried out for using a closed reactor for wastewater applications [17,37].

3.1 Effect of Geometry

Under ideal conditions for the closed channel reactor, there is a complete mixing of the water flow inside the reactor, i.e. plug flow, which will lead to equal distribution of the UV dosage. This, however, is not possible in real flow conditions because the flow of particles inside the reactor is unique and thus will receive unique dosage. Hence, the calculation of the UV dosage is in terms of distribution rather than a fixed value [2]. There are various hydraulic features, which affect the dosage received by the water. One of the easiest changes made includes the inlet and outlet location. Offsetting the reactor inlet and outlet leads to better mixing of the water [25]. Based on inlet-outlet location, there are different types of reactors such as L type, reverse L type, linear type, and U type. The L type reactor has the inlet perpendicular to the axis of the reactor while outlet is parallel. Reverse L type has an inlet parallel and outlet perpendicular to the axis of the reactor. The linear type has both inlet and outlet parallel to the axis of the reactor. U type of reactor has inlet and outlet both perpendicular to the axis of the reactor. U type and L type are more turbulent compared to the other two because of the perpendicular inlet. L type of reactor performed better than the U type of reactor for set conditions in terms of fluence distribution. Geometrical changes brought different results in terms of distribution and treatment of water. Changes in the dimensions of the reactor introduce changes in the dosage received by the water. While in general, the increase in the length of the reactor and decreasing the cross-section area of the reactor improves the reactor performance for the U type reactor. Figure 2 shows different type of inlet outlet location as discussed above. [73].

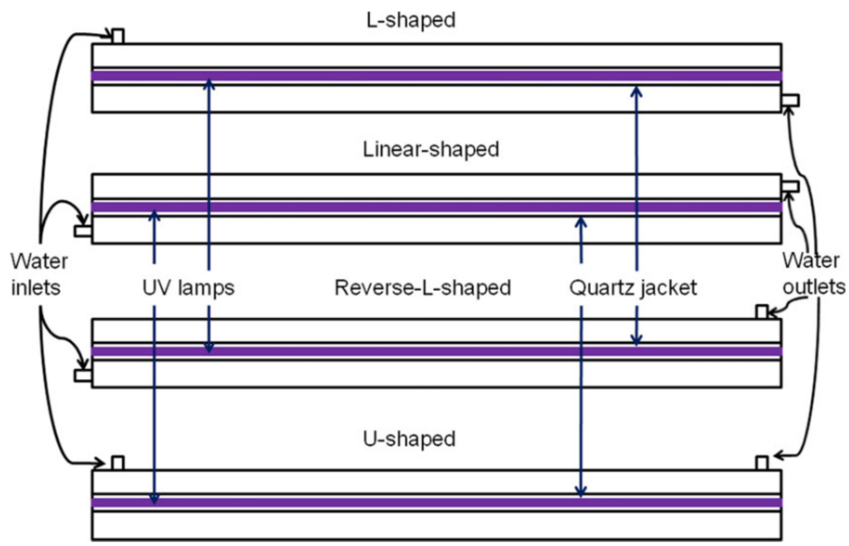

Figure 2: Layout of single lamp UV photo reactor

Changes in the shape of the reactor can remove dead zones (areas that receive no dosage). Accomplished by flattening the reactor instead of the complete circular reactor. Such an improvement in the reactor can lead to reducing 37% of the lamp output for a similar dosage [74]. Similarly, changes in the upstream hydraulics can also affect the dosage. 90 degree bends perpendicular and parallel to the reactor axis upstream of the reactor inlet are less efficient compared to the pipe straight to the inlet reactor [29]. Roughness of the wall produces effects not only on the hydraulics of the system but also on the dosage and RED values of the reactor. There is a drop in the velocity with an increase in the roughness value of the pipe. Compared to the smooth pipe, a rough pipe increases the value of RED depending upon the Reynolds number of the flow. At lower Reynolds numbers, there is a higher percentage difference between the smooth and the rough surface [33].

The above methods rely on improving the system's geometry to achieve the required amount of dosage and in addition, achieved by using reactors in series. The theoretical evaluation of reactors in the series concludes that the dosage received by two identical reactors is twice the single reactor's dosage. Hence, for treating the microorganisms, which requires two times the RED value of a single reactor, can be treated using two reactors in series [72].

Open channel reactors have different challenges to the closed channel reactors in terms of hydraulics of the system. As open channel reactors are mainly for wastewater applications, UVT of the water is less than 70%. UVT has an exponential relationship with UV sensitivity; hence, the treatment of highly insensitive microbes does not improve with an increase in UVT. Thus, it is better to decrease the distance between the lamps to treat the microbes with higher sensitivity than to increase the UVT. Like the closed channel reactor, roughness also affects the open channel reactor. However, these effects are negligible for higher Reynolds numbers. Analysing the open channel reactor requires a large amount of computational power. However, these simulations are more cost-effective than experiments. De featuring the geometry can simplify the model. A simple geometry consisting of channel and lamp provided very close results to a full-scale geometry consisting of all reactors' features. The use of this can decrease the complexity and cost of the simulation [17,31,37,60].

3.2 Effect of lamps

Closed channel reactors classified as parallel and perpendicular reactors, based on the arrangement of the lamps. A system with lamps perpendicular to the reactor axis is classified as perpendicular reactors while a system with lamps parallel to the axis of the reactor is classified as parallel reactor. The effects of different configuration are complex and dependent on several different other hydraulic factors. When compared to similar UV dosage and a similar number of lamps, parallel lamp configuration provided better log reduction compared to the perpendicular lamp configuration. These factors are highly sensitive, with small changes in location and configuration results in different dosage. For example, a similar number of lamps and parallel configuration, but with two different orientation types, leads to different log reduction results. Lamps placed under the inlet-outlet have better log reduction compared to the evenly distributed lamps inside the reactor [62,73]. The use of a genetic algorithm methodology can achieve arrangement optimisation. This algorithm finds the optimum location and arrangement of lamps inside the reactor for the highest minimum value of RED. The calculation for the optimum lamp circle uses the following formula: $\frac{D_c}{2} \pm 20\,units$. Where D_c is the diameter of the reactor. In addition, the asymmetric lamp arrangement shows better results than symmetric arrangement in terms of dosage received by the microorganism. Research shows that asymmetric arrangement improves RED value by 15%. The relationship between the lamp arrangement and RED is quite complex, hence the use of genetic algorithm methodology to find the optimum arrangement inside the reactor [34,36]. Turning off lamps one by one, can establish the importance of each lamp. Turning off the lamps without removing them from the reactor to maintain similar hydraulics and flow pattern inside the reactor. Using this technique, it is found that the lamps closer to the main flow are more effective than the lamps away from the main flow for the overall dosage received by the reactor [22].

A single lamp with equivalent power to six lamps performs better than six lamps. The reason for this is because of the higher power and the barrier effect. Increasing the flow rate due to the hydraulic pressure can minimise the barrier effect. There is the use of multi reactors in industrial scale for large cross-sections. Similarly, research indicates that the single lamp reactor's energy distribution is better than the double lamp reactor, while the volume emission rate is similar. However, two lamps have better irradiation near the walls compared to the single lamp [71,73].

Using an online monitoring system can optimise the number of lamps and the configuration of the lamps. Monitoring three factors, including the lamp output, attenuation coefficient, UV transmission of the water and quartz sleeve-fouling coefficient. The data collected from this could help in improving the efficiency of the system in real-time by changing the power of the lamps. In addition, it determines the accidental breaking of lamps inside the water or cleaning required inside the reactor. The increase in the lamp power increases the dosage received by the microorganisms [8,13].

Open reactors are again subdivided into two types based on the configuration of the lamps arrangement inside the open channel reactor: 1) horizontal configuration and 2) Vertical configuration. The horizontal configuration is advantageous over vertical configuration in terms of residence time for the microorganism. This is because the flow of water is along with the lamps [17]. However, the research presents contradictory results that the vertical lamp configuration performed better than the horizontal lamp configuration. In addition, staggered lamp positioning is better than parallel lamp positioning in terms of RED value received by the water. The differences in the value of the RED for vertical and horizontal configuration is more at lower Reynolds numbers [37].

3.3 Effect of temperature

There is no temperature effect on treating the water or on the hydraulics of the system if there is a continuous flow of water with small variation in the inlet temperature [22]. However, if there is a significant increase in the water temperature, then relative UV intensity increases from 0.53 at 4.7-degree Celsius until approximately 32 degree Celsius to 1.26 after that temperature decreases. This could have a significant impact if the temperature of the inlet water varies widely during different seasons. The use of other factors such as varying flow rate inside the reactor can offset the effect of the temperature [13]. However, it is worth noting that for three different inlet temperatures of 20, 30, and 90 degrees, there is a very small change in the value of RED. Thus, for the majority of the simulations, temperature effects are neglected [22].

3.4 Effect of UVT

Drinking water applications have UVT higher than 70% while wastewater application usually has UVT less than 70%. Higher UVT of the water improves the dosage received by the microorganism because the fluence rate inside the reactor increases exponentially with an increase in UVT. Increase in UVT also leads to better energy distribution inside the reactor [8,71]. Flow rate must be lower for lower UVT to allow higher residence time for the particle while, at higher UVT values, the flow rate is higher [69].

3.5 Effect of flow rate

The flow rate is an essential parameter while considering the hydraulics of the reactor. Ideally, if a reactor can treat all the water that flows in it, then the flow rate should be as high as possible to obtain maximum efficiency out of the system. However, due to the limitations of the reactors, it is not possible to attain this. Hence, it is very important to determine the ideal flow rate for each system. It is not possible to carry out experiments for every change in flow rate. Hence, CFD is a vital tool in determining the flow rate of the system. Current systems use different flow rates ranging from as low as 1 m^3/h up to as high as 552 m^3/h. Low flow rates are generally used for laboratory-scale experiments where the models are scaled. Industrial-scale models use higher flow rates. Published research indicates the considerable amount of laboratory-scale model tests carried out. However, for the industrial-scale models, such information is scarce.

Higher Reynolds numbers decrease the RED value, which is because there is less residence time for the particle. At low Reynolds numbers, flow approaches laminar flow; this leads to too little to no mixing of flow inside the reactor. At low Reynolds numbers, (usually corresponds to a low flow rate) the flow is laminar. At such a low flow rate, there is little mixing of the flow. This leads to an inefficient system, as the UV dosage is not uniformly distributed. At higher Reynolds numbers there is proper mixing because of the swirl caused inside the reactor. This leads to a better mixing of water [25]. CFD used to determine the ideal flow rate for each reactor. Each reactor because of its uniqueness provides a different ideal flow rate to the system [19, 72]. Water profile plays an important role, including the determination of the dosage inside the reactor. With changes in the internal reactor profile, there are changes in the water profile. This, in turn, affects the path of the microorganism. Due to such effect, the flow velocity is higher with lower turbulent velocity in the parallel reactor compared to the vertical reactor.

The significant effect of hydraulics as well as the models used for the determination of the dosage it has become apparent that it is essential to understand both the assumptions and the limitations of the model. The method employed by researchers for the determination of the optimum flow rates for the given reactor is to initially find the optimum configuration using a constant flow rate and then using this optimum configuration to find the optimum flow rate [36]. Table 4 summarises all the effects on the UV systems.

Table 4: Comparison of the type of effects on the UV systems

Type of effects		References
Geometrical effects	Closed Channel	[22,33,34,37,69,72]
	Open channel	[13,17,31,37,68,76]
	Not mentioned	[2,13,62,72,73]
Effect of lamps		[15,22,33,34,36,37,40,42,44,49,50,56,59,61,62,67–69,71,74]
Effect of Temperature		[15,23]
Effect of UVT		[7,8,21,29,41,71]
Effect of Flow rate		[7,13,14,25,27,30,34,36,39,41,43,57,74,78–80]

4. Scope of UV treatment

DWI (water regulatory company of UK) research indicates that only 10% of current water companies use UV treatment process. Research in 2017, shows that 1492Ml/d amount of water is treated using UV light from 139 units [81]. Thus, there is massive scope for the further development of the UV treatment process. As highlighted in the paper, the current system uses mercury lamps as the source of UV light for treating water at a commercial scale. Several disadvantages of mercury lamps have led to LED lamps' development as a source of UV light. The United Nations Environmental Program (UNEP) has drawn the 'Minamata Convention', which has as one of its goals the phasing out of mercury and all mercury-related products. Although this convention does not directly mention UV-Mercury lamps, it does signal the global initiative of phasing out the usage of mercury [82]. Table 5 summarises the advantages and disadvantages of the mercury system against the LED system. Wide range of research has proven LED at bench scale to be effective in disinfecting water [6]. Recently there is advancement in terms of developing the first full-scale UV-LED drinking water disinfection. This full-scale LED-UV treatment plant is being used for municipal water treatment work and is equivalent to the mercury-based UV treatment in terms of water quality [52].

Table 5: Comparison of Mercury lamps vs LED lamps

	Mercury Lamps	LED lamps
Material	Usage of very toxic material	No issues as such in LED lamps
Response time	It takes time to heat up mercury lamps	They operate quicker and do not have any lead time
Energy efficient	Less efficient	More efficient
Life span	Shorter life span	Long life span
Carbon footprint	Bigger carbon footprint	Comparatively smaller footprint

5.Conclusions

Mercury lamps have been dominating technology in UV treatment process so far. The CFD models are pivotal and decisive in the development of the UV technology. The CFD models can predict the dosage received by the water considerably better than just applying the average dosage to the system based on the power of lamps. Using CFD models and the fluence model benefits the flow prediction and unlocks the opportunity to optimise the model for its most efficient application. The limitations and the disadvantages of the current commercial system has paved way for the research in the LED lamps as a source for the generation of UV light. More research is required for the development of LED lamps capable of handling a large quantity of water.

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