The on-going development of a CFD model to better understand the plasma arc discharge in a waste-water treatment application

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Abstract: The generation of plasma discharge in water can be used for environmental pollution control. A Computational Fluid Dynamics (CFD) model is used to study the relevant chemistry and fluid dynamics encountered when plasma is generated. A staged approach is used to create the CFD model which initially only considers simple physics. More detail is then added to the model which includes electromagnetic and plasma models.

Keywords: arc discharge, low current, non-thermal plasma

1. Introduction

The degradation of hazardous organic pollutants in water is one of the critical and urgent topics in environmental research. Advanced Oxidation Processes (AOP's) have been traditionally used for the generation of highly reactive species, especially hydroxyl (OH) radicals. There are several AOP's which generate OH radicals, however these methods are known to be slow [1].

Non-thermal plasma is an emerging technique in environmental pollution control technology and is considered to be an AOP. The plasma is produced by a high voltage discharge process resulting in the generation of a large amount of high energy electrons and active species such as active radicals and molecules. Compared to conventional AOP approaches, non-thermal plasma can achieve a greater output and better efficiency [1].

Since plasma based water purification is an emerging technology, critical reviews by previous researchers have identified certain focus areas for further and extensive research in order to develop effective applications for future use. It has been suggested that Computational Fluid Dynamics (CFD) can be used to study the relevant chemistry and fluid dynamic effects at the plasma-liquid interface [2]. Therefore, this work presents a 3-D turbulent model being developed for understanding the arc discharge behaviour between two electrodes submerged in the liquid phase.

2. Plasma in contact with liquid water

Placing a plasma in contact with liquid water drives the advanced oxidation in the solution. The most direct method of generating a plasma in water is referred to as the direct discharge method. In this method, the electrodes are immersed in liquid water in what is referred to as a pin-to-plane reactor arrangement. When the applied electric field of the electrodes reaches the desired conditions, an arc discharge will form between the electrodes. A photograph of a typical arc discharge is shown in Fig. 1. This arc discharge is the source of the reactive oxygen species. The direct discharge also produces shockwaves and ultraviolet, both of which can drive decomposition and ultimately the destruction of organic contaminants in solution, including microorganisms [2].

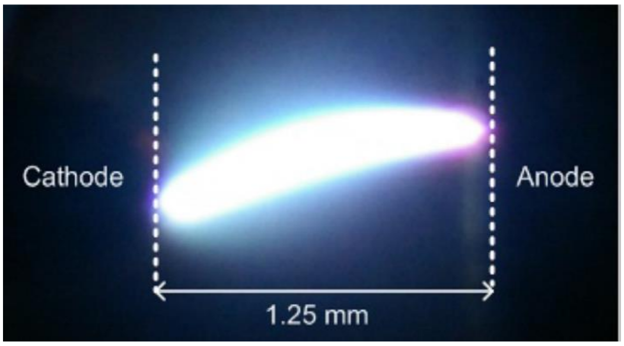

Fig. 1. A typical arc discharge [3].

3. Computational modelling approach

It is intended that the final CFD model will include multi-physics (air and water), electromagnetic and plasma physics. A staged approach will be utilised which will initially begin with a simplified model, with the complexity being increased as the model is further developed. This paper will focus on the establishment of the simplified model.

STAR-CCM+ version 13.04.010 has been used to create a CFD model of a plasma reactor which is of the pin-to-plane configuration. STAR-CCM+ is a Computational Aided Engineering Solution for solving multidisciplinary problems in both fluid and solid continuum physics, within a single integrated user interface. The software will be used to carry out all stages of the engineering analysis which will include:

- Import of the computational domain
- Mesh generation
- Solution of the governing equations
- Analysis of the results

4. Constructing the volume mesh

The construction of the volume mesh has a direct influence on how accurately STAR-CCM+ simulates fluid flow and energy. The mesh will influence the rate of convergence as well as the accuracy of the final solution. The mesh has been designed in order to provide adequate resolution in regions where spatial gradients are expected to be high [4]. In this CFD model, such a region is expected to be the inter-electrode gap.

In this inter-electrode region, the plasma will come into contact within liquid water and the physics is expected to be highly dynamic and transient. Discharges in a liquid typically require a rapid breakdown process, which in most cases is electrically driven by strong electric fields. The complex processes which need to be considered when a plasma comes into contact with liquid water include gas phase chemistry, multiphase species transport, heat and mass transfer, interfacial reactions and liquid phase chemistry [5].

The constructed volume mesh as well as the definition of the different regions is shown in Fig. 2. Note that a converging section has been added to the Air Outlet region. This is done in order to accelerate the flow out of the computational domain and prevent any unnecessary reversed flow errors.

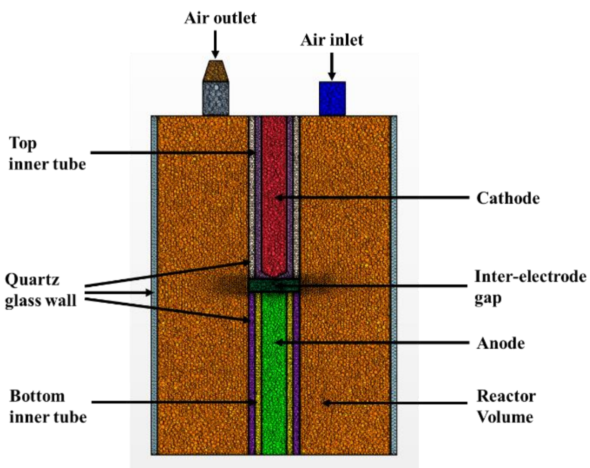

Fig. 2. Volume mesh.

The volume mesh has been constructed using the polyhedral mesher model. Polyhedral meshes are relatively easy and efficient to build, requiring no more surface preparation than the equivalent tetrahedral mesh. A polyhedral mesh will contain approximately five times fewer cells than a tetrahedral mesh for a given starting surface. The polyhedral meshing model utilises an arbitrary polyhedral cell shape in order to build the core mesh. The polyhedral cells that are created typically have an average of 14 cell faces [4].

The prism layer mesh model was used in conjunction with the polyhedral model to generate orthogonal prismatic cells next to wall surfaces and boundaries. This layer of cells is necessary to improve the accuracy of the flow solution. Prism layers allow the solver to resolve near wall flow accurately which is critical in determining not only the forces and heat transfer on walls, but also flow features such as separation [4]. A cell base size of 0.8 mm was selected for all regions, except for the inter-electrode gap, where a cell base size of 0.2 mm was selected. An enlarged view of the inter-electrode gap is shown in Fig.3. The smaller mesh size in this region can be clearly seen compared to the other regions.

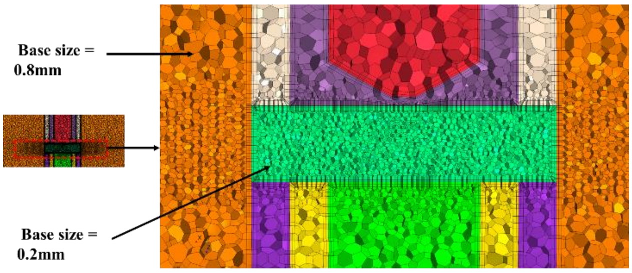

Fig. 3. Enlarged view of the inter-electrode gap.

5. Selecting physics for the simplified model

In actual operation, air is supplied at both atmospheric temperature and pressure, i.e. 298.15 K and 101.325 kPa respectively. The mass flow rate of air entering the plasma reactor is 0.000197 kg/s (10 l/min). The reactor volume will contain approximately 80% water at a temperature of 313.15 K. The reactor contains an air outlet region open to the atmosphere. There is also a water outlet region at the base of the plasma reactor which is only used for drainage after the reaction. The water outlet region will remain closed during operation of the reactor and is therefore not included in the volume mesh.

For the simplified model, only air will be selected to pass through the reactor. This is done in order to reduce computational complexity and confirm that the velocity vectors pass through the computational domain as expected.

The fluid flow is expected to be turbulent and will therefore be characterised by irregularly fluctuating flow quantities. These fluctuations will be at such small scales and high frequencies that resolving them in time and space comes at excessive computational costs. Rather than solving for the exact governing equations of turbulent flows, it is less computationally expensive to solve for averaged or filtered quantities and then approximate the impact of the small fluctuating structures [4]. The turbulence model chosen will be of the type that provides closure for the Reynolds-Averaged Navier-Stokes (RANS) equations.

The turbulence model chosen is the K-Epsilon turbulence model which is a two-equation model that solves transport equations for the turbulent kinetic energy (k) and the turbulent dissipation rate (ε) in order to determine the turbulent eddy viscosity [4].

The coupled flow model was chosen to solve the conservation equations for mass, momentum and energy simultaneously using a pseudo-time-marching approach. An advantage of this formulation is its robustness for solving flows with dominant source terms. Another advantage of the coupled solver is that computational time scales linearly with cell count, i.e. the convergence rate does not deteriorate as the mesh is refined.

A velocity vector plot calculated from the simplified model is shown in Fig. 4. The velocity vectors follow the expected path indicating early confidence in the constructed computational domain and volume mesh.

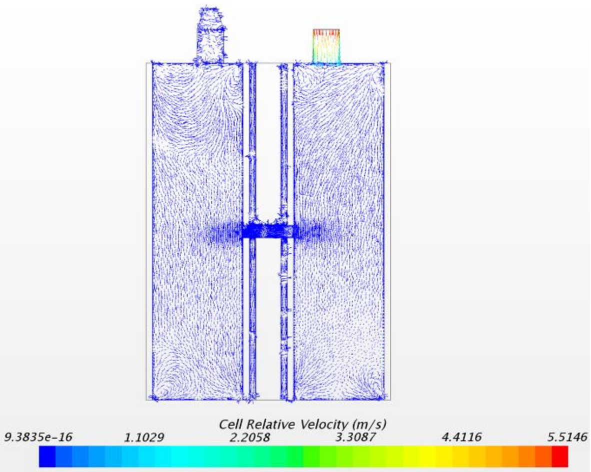

Fig. 4. Velocity vector plot.

6. High Performance Computing (HPC)

High Performance Computing (HPC) is necessary in the analysis of complex flows using CFD since it allows for problems to be tackled within realistic time scales or it allows for new problems to be explored. HPC makes use of parallel processing for running advanced application programs (such as CFD models) efficiently, reliably and quickly. HPC in recent years has been justified by the advances made in computing performance, combined with the increased availability of large-scale computing resources [6].

The resources available at the Centre for High Performance Computing (CHPC) located in South Africa are utilised for solving the computational model. The CHPC comprises of a DELL cluster that has the ability to perform at petaFLOP levels. In computing, floating point operations per second (FLOPS) is a measure of computing performance. The cluster can be defined as a group of tightly coupled computers working in unison which communicate using a high performance interconnect. The specifications for the Lengau cluster are provided in Table 1.

Table 1: Lengau cluster specifications.

System Name	**Lengau cluster**
CPU	Intel ® Xeon ®
CPU clock	2.6 GHz
CPU cores	32832
Number of nodes	1368
Memory	148.5 TB
Theoretical peak performance (Rpeak)	1.307 petaFLOPS
Maximal achieved performance (Rmax)	1.029 petaFLOPS

A Secure Shell (SSH) is used for logging into the cluster and a Secure Copy (SCP) command is used to transfer simulation files between the local computer and the cluster. A job script is prepared in order to submit the simulation to the cluster. A Portable Batch System (PBS) job scheduler will assign the simulation file to the appropriate que and machine. The openSUSE Linux based operating system has been used in this case to communicate with the Lengau cluster.

7. Modelling the plasma arc

STAR-CCM+ allows for the modelling of plasma arcs. This type of plasma consists of highly ionised particles which are generated when a large current of high voltage creates an electric arc between two electrodes. As this electric arc passes through a gas, the gas particles are heated strongly and become ionised.

Since the particles are ionised strongly, chemical equilibrium is assumed, and due to the frequent collisions of particles, the electrons remain in thermal equilibrium with the gas temperature. However, it is possible that the particles are in non-thermal equilibrium near the electrodes or walls.

The computational domain is modified to include a 0.2 mm diameter initial hot channel in the 1 mm inter-electrode gap (see Fig. 5). This hot channel has an initial temperature of 11000 K and will serve the purpose of igniting the plasma.

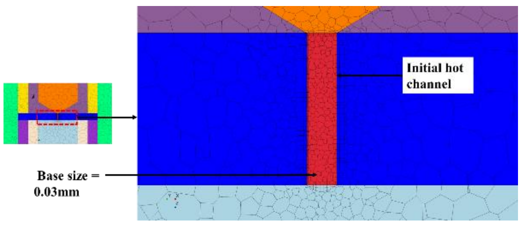

Fig. 5. The initial hot channel.

The Implicit Unsteady model is chosen for modelling time with a time step of 0.1 µs. The Implicit Unsteady solver will have the primary function to control the update at each physical time for the calculation.

The Equilibrium Air Model will be chosen to compute the density and density derivatives with respect to time and pressure. This model is well suited for air plasma with temperatures that are below 25000 K.

The Electrodynamic Potential model calculates the electric potential due to electric currents. An initial condition electric potential of -3000 V will be applied through the initial hot channel.

The Electric Current model is selected to define a total electric current of 0.4 A through the inter-electrode gap boundary. The Two-Way Coupled Magnetohydrodynamic (MHD) model accounts for the interaction between the electrically conducting air and the magnetic field. The Ohmic Heating model is used to solve for the heat which is generated in the conducting air due to the flow of electric current. This effect is also referred to as the Joule effect.

8. Discussion

The first 15500 iterations of the calculation equate to solving a physical time of 0.00003 s. The temperature and electric potential profile of the arc at this physical time are given in Fig. 6 and Fig. 7 respectively.

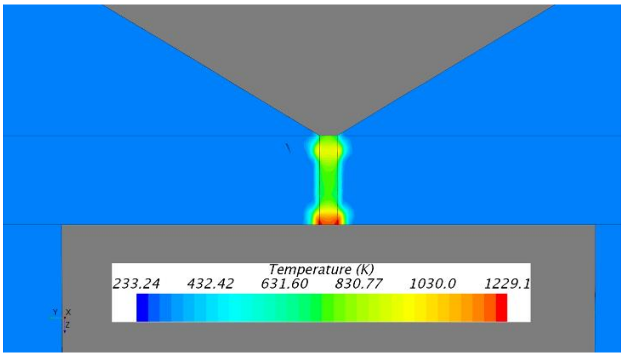

Fig. 6. The arc temperature profile.

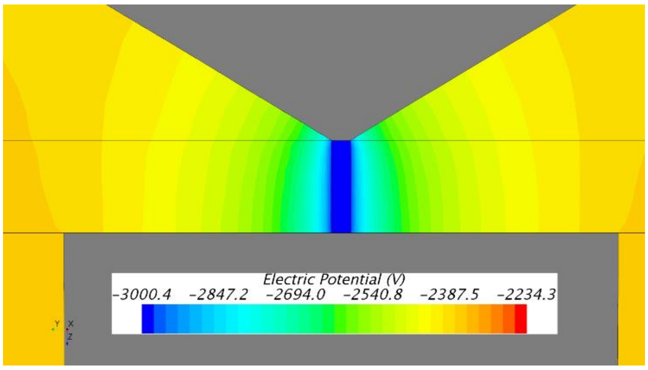

Fig. 7. The arc electric potential profile.

The temperature profile shows that the CFD model is able to spark the plasma in the initial hot channel. The hottest point is currently being observed at the anode, however it is expected that the hottest point should be observed at the tip of the cathode. The electrical conductivity for air at 11000 K and 101.325 kPa is 4390 S/m, which has been input into the model. Future work will involve customising the initial hot channel air parameters further by defining values such as Magnetic Permeability, Scattering Coefficient and Turbulent Prandtl Number. It is possible that these parameters may impact the calculation of the temperature profile.

The electric potential profile shows a uniform electric potential in the initial hot channel between the electrodes. However, it is expected that there would be a drop in electric potential between the cathode and anode. Further analysis of the electromagnetism model is required to fully understand the calculated electric potential profile.

9. References

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