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MODELLING OF RECTANGULAR SEDIMENTATION TANKS

Report to the WATER RESEARCH COMMISSION

by

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CFD yields so much information, and it has to be viewed as graphics in colour or grayscale tones to comprehend, most of the graphics in chapters are not included in the text. To include it would have made the report too bulky and expensive. Instead it is provided on the CD ROM as files that are referred to in the text and can be opened on the computer for viewing.

EXECUTIVE SUMMARY

MOTIVATION FOR STUDY

Sedimentation tanks are the workhorses of any water purification process. It is thus crucial for the sedimentation tank to be operated to its full potential. It is not only the chemical aspects of flocculation that cause problems, however. Hydraulics also play a prominent part. Overdesign of plant is common, leading not only to unneceassary capital expenditure, but also to water wastage in the form of excessive sludge. Inadequate design causes overloading of filters, leading to frequent backwashing which also wastes a significant percentage of treated water. Many plants are already a few decades old and do not incorporate the latest developments in technique, e.g. inlet design. Sedimentation tank performance is strongly influenced by hydrodynamic and physical effects such as density driven flow, gravity sedimentation, flocculation and thickening. In turn the velocity and density patterns in tanks influence these processes and are therefore of great interest to design engineers.

The primary performance indicator for sedimentation tanks is the fraction of the solids present in the raw water removed by the sedimentation step. However, the absolute percentage is not sufficient – an overdesigned tank will remove a large percentage without being really efficient. Therefore it is necessary to qualify it in terms of the design capacity. It must also be qualified in terms of the smallest size of floc particles that will still be removed by it.

Computational Fluid Dynamics (CFD) is the analysis of systems involving fluid flow (gases or liquids) by means of computer-based simulation. It is a research tool and a design tool and it is complementary to theory and experiments. CFD can also be described as a method to investigate and simulate fluid flow by means of iterative calculations on computers. It was developed originally to study aerodynamics, but has since been applied to many different types of flow under a great variety of conditions. A recent application (since ca 1990) is to use it for the simulation of unit processes in water treatment, e.g. chlorine and ozone contactors, sedimentation tanks and sludge thickeners.

The basic technique utilized in CFD is to divide the region or component in or through which the flow is to be investigated (the flow domain) into a grid of thousands of small blocks. Boundary types and conditions for the domain (inflow, outflow, pressure, symmetry), values for inflow (flow rate, concentrations, temperature) and physical values for the fluid (density, viscosity) are specified. The computer then calculates values for velocity components, pressure, momentum, energy and concentrations for each cell iteratively until the values converge for a steady state solution, or for a required number of iterations that yield sufficient accuracy for nonsteady flow cases. The results can then be visualized by displaying it graphically by looking at views (slices) through the flow domain, for example as velocity vectors, pressure contours or particle tracks. It can also be imported into applications like spreadsheets for further mathematical analysis.

The application of CFD to the simulation of sedimentation tanks is fairly recent because it involves modelling of the movement of solid particles in water, i.e. twophase flow. This increases computer memory and processor speed needs. With the advent of PC's with processor speeds in the Giga-Herz range and Gigabytes of RAM it has become feasible and has put CFD as a tool within the scope of standard consulting practice in the design and operation of water purification and treatment works.

RESEARCH OBJECTIVES

- Evaluate the suitability of CFD as a technique for design and research of rectangular sedimentation tanks.
- Design CFD models for simulation of sedimentation tanks, i.e. grids and numerical descriptions.
- Validate the models with experimental data.
- Use CFD to investigate the effects of design parameters and operational parameters.
- Make recommendations for improved design and operation of sedimentation tanks.

The study was conducted in three stages. First a model was developed to compare with results published for a clarifier at a sewage treatment plant at Jönköping, Lund, Sweden. This clarifier is well studied and often used for benchmarking. It also enabled the research workers to become proficient with the Flo++ CFD package that was used for this project, as well as with the technique of developing a suitable grid for the model, which is the most time-consuming aspect of CFD modelling.

This was followed by experiments with a physical, small-scale (100 l) perspex model of a rectangular sedimentation tank. (Hereafter it will be referred to as the labtank.) It was used to provide information for validation of CFD models of it. In order to obtain realistic experimental results, it was necessary to test a number of substances for the simulation of the floc particles. Finally ground and sieved crystalline polystyrene was used.

Finally, a CFD model was developed to simulate the full scale rectangular sedimentation tanks at the Midvaal purification works near Orkney.

The CFD simulations of the laboratory model and the Midvaal tanks were done by setting up standard cases for each, *i.e.* a configuration and operating conditions that represented the physical tanks as they were built, and then varying different aspects of the configuration or operating conditions one or two at a time to determine the effect. Only type 1-settling (discrete particles in dilute suspension) was simulated, as it is the applicable type for the operating conditions in rectangular sedimentation tanks foir potable water treatment.

CONCLUSIONS

From the results of the various investigations and simulations the following conclusions can be made:

CFD has reached a level of development where it has become a useful tool for research, design and operation in water technology. It is now possible to use standard software packages and desktop computers to analyse and investigate fairly complex situations in terms of configurations and conditions within reasonable time periods and at lower cost than doing experimental work. Very realistic models that mimic nature in such a way that the behaviour of the models cannot be distinguished from that of the physical systems they are modelling can be developed. Such models can

therefore be used with confidence to investigate the characteristics and behaviour of the physical systems, including the effects of changes in or to it.

The realism of the CFD models developed in this project did lead to valuable insight into the real dynamics of the tanks. For example, it was observed that the systems studied were behaving non-linearly (i.e. chaotically) at higher temperatures in both the numerical CFD and the physical laboratory models. In another case removing some sumps in a model of the Midvaal tanks showed that a configuration modification that was intuitively expected to simplify the dynamics of the tank, would instead cause it to become significantly less stable and robust and thus susceptible to changes in operational conditions.

The results of the physical experiments and CFD simulations done showed that the presence of the solid phase, *i.e.* floc particles, in the water affected the dynamics of sedimentation tanks. Therefore two-phase simulation will normally be required to obtain realistic information for design and operational purposes. To do two-phase modelling the solid phase can be simulated as either another fluid (*i.e.* sludge) completely mixed with the water entering the tank, known as the scalar approach, or as discrete solid particles. Both approaches have their own advantages and disadvantages. Discrete particle tracking yields more information about the interaction of the water and the particles and insight into the development of the flow patterns than the scalar approach. It is computationally much more intensive and time consuming and is unnecessary if the modeller is not particularly interested in the particle trajectories. It is also almost impossible to use it to calculate solids concentration in the outflow, since one needs a very exact particle size distribution to do so. The scalar approach can do this much easier.

The complexity of the computational grid of cells used for the CFD simulations always requires a that a balance be struck between the resolution required and the computational requirements. In order to obtain mesh-independent solutions that are realistic simulations of the physical reality the grid must be as detailed and as fine as possible, but to optimise time frames and hardware requirements as few cells as possible must be used. Detailed grids must be developed for inlets and outlets, i.e. the

grid must be refined in these areas. The same should be done for any area with large variations in velocity, e.g. vortices.

It was found that the physical characteristics of the flocs (size, shape, density, concentration and composition) are not such significant parameters in the operation and performance of sedimentation tanks used for potable water treatment as originally assumed, due to the much lower solids concentrations and greater particle size distributions than those encountered in sewage water treatment.

In order to obtain information on floc particle composition, solids present in the Mooi River in Potchefstroom was flocculated by means of conventional jar tests with different metal hydroxides as coagulants. The flocs formed were observed under a microscope to determine their composition in terms of the different types of solid material suspended in the water. All the flocs observed consisted of a random mixture of the mineral particles, bacteria, algae and diatoms present in the water. The extent of this work is too little to make any definite or final conclusions, but it does show that floc composition will tend to be very variable, depending on seasonal and environmental conditions. This implies that when designing actual tanks, a large variation in floc particle composition (and therefore size, density and shape) must be considered - at least the possible extremes and typical values of mineral and microbial content. More research into this aspect is recommended.

A set of criteria were compiled for suitable floc simulants in physical experiments and a number of substances were tested viz. synthetically prepared flocs, sago grains, maize meal and, finally, ground polystyrene granules. The latter was found to be ideal in all respects and is recommended to any future researchers.

The ability of sedimentation the tanks to clarify water by letting suspended solids settle out as flocculated particles depends on two aspects: (a) The water flow pattern through the tank, which in turn is determined by the configuration of the tank and by operational parameters (solids concentration, water flow rate and temperature). (b) The settling characteristics of the particles as determined by their shape, size and interaction with the water through drag and buoyancy forces. Water flow patterns dominated particle settling in determining the dynamics and efficiency of rectangular

sedimentation tanks experiments and imulations done in the project. It was also observed that the water flow patterns were remarkably stable and robust for any particular configuration. With regard to the water flow pattern through tanks it was found that the most important aspect was the design of the inlets, especially their placement.

The experiments and CFD simulations showed that baffles were not necressarily effective to dissipate kinetic energy and prevent short-circuiting between inlets and outlets. Putting baffles at the inlets did not affect flow patterns or particle trajectories through a tank as a whole or at the outlets specifically. Neither did it affect particle settling patterns on the bottom of the tank. The baffles did have a significant effect on the vortices and particle trajectories directly at the inlets. The vortices were split up into more vortices and the density waterfalls became steeper between the baffles and the inlets. This can have an effect on the flocculation and settling of real floc particles in practice because more vortices and higher velocity gradients at the inlets were observed to capture more of the floc particles and recirculate them. This effectively forms a sludge bed or blanket in inlet zone. Further research into this aspect is recommended.

The hydrodynamic parameters were much less important than expected. (*I.e.* the water flow rate and velocity components in the different axial directions.) The position and relative velocities of the inlet vortices changed to an extent, but the basic flow patterns remained the same. Temperature, which affects water viscosity and density, did not affect the flow patterns, but did affect the stability of the flow and the settling behaviour of the particles.

Outlet configuration is generally assumed to influence the flow significantly due to short-circuiting, but was found to have minor effects on flow patterns and particle trajectories. Only minor differences were observed in flow patterns and particle trajectories in the inlet and settling zones, whether the outlets were in the form of systems of distributed outlet channels, or overflow weirs at the back of the tank, or even merely a holes in the back walls of the tanks.

The presence of the settling particles themselves also affected the flow dynamics. Due to their interaction with the water through drag and buoyancy, they cause the development of density waterfalls in inlet zones. The extent to which this happened depended on the concentration of the particles. Without particles in the inflow streams the water flow patterns in the simulations and labtank model experiments invariably developed direct shortcuts between the inlets and the outlets. With particles, the flow patterns were more complex because the particle-induced density waterfalls interacted with the inlet vortices.

As far as floc particle settling behaviour is concerned, the water flow patterns in the tank had the most significant effect. This mostly stems from the development of density waterfalls.

Water temperature did affect tank efficiency in the physical labtank to an extent which is usually not considered in the design of the tanks. The increased viscosity and density of water at the lower end in the normal operational temperature range of 10 to 25 °C caused significantly larger fractions and sizes of the particles to be washed out of the tank via the outlets. The Flo++ models of the labtank and Midvaal tank also showed an effect on the particles, but very much less so than in the case of the physical tank. However, the water temperature did have a significant effect on the numerical behaviour of the models. At the lower temperatures $(4 - 15 \, ^{\circ}\text{C})$ the models converged much more quickly than at the higher ones $(15 - 25 \, ^{\circ}\text{C})$. In the case of the labtank, the CFD models ususally did not converge at all at the higher temperatures, but could only be solved as unsteady cases. Again, it is an open question for further research whether this instability is due to numerical or physical reasons, or both.

The conventional approach for the design of sedimentation tanks is still valuable as a tool for the first stage of tank design to obtain general conceptual information, but such a design should then be subjected to a rigorous CFD analysis of the its configuration and of the effect of changes in operational parameters. Apart from the obvious benefits of proper understanding of tank dynamics and optimization of design, overdesign is wasteful and can be detrimental, because clarified water in the vicinity of the outlets is an ideal medium for algal regrowth.

Another aspect for further research to come out of this project is what contribution the high-velocity vortices in the inlet zones make to effective clarification in practice. They trap particles, effectively forming sludge blankets where the particles can flocculate further, or simply recirculate until they move into a lower velocity region from which they can settle out. Could this effect be enhanced by increasing the intensity of the density waterfall?

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TERMINOLOGY

The usage of terminology in the scientific literature related to this research project is not always consistent. For clarity and consistency the usage of terms in this document will be as follows:

Coagulation; flocculation

These two terms are often used interchangably but the practice of some authors to distinguish between them will also be followed in this document. Coagulation is thus defined as the process of charge neutralization and colloid destabilization. Flocculation is the agglomeration of the destabilized colloidal particles into larger settleable particles.

Clarification; settling; sedimentation; thickening

The term clarification is also a broad one and is often used interchangably with the terms settling and sedimentation. In this document the term will be used as an inclusive one for processes that results in the physical removal of particulate material from water, including sedimentation (settling), flotation and sludge thickening, but excluding filtration. (Although filtration is strictly spoken also a clarification process, it is considered and treated as a separate consecutive step in conventional water treatment, rather than an alternative or complementary one.)

Thickening is used when the primary purpose of the tank is to concentrate the solids in the water, e.g. in wastewater treatment, where the sludge is concentrated for recycling or disposal.

The terms tank and basin are also used synonymously by authors. In this document tank will be used, except when quoting directly from a source.

The terms sedimentation and clarification are used interchangeably with regard to preparation of potable water, although there are some subtle differences in the connotations. Sedimentation may be classified into various types depending on the characteristics and concentrations of suspended materials (Peavy et al, 1985: 114). In

this document the process will be referred to as sedimentation (and occasionally settling) and the physical equipment as as tanks or sedimentation tanks.

Model

In general, a model is a representation of an object or process. The representation can be physical (e.g. a scale model), conceptual (e.g. an analogy) or abstract (e.g. a set of mathematical equations). In this project the term is used in two ways:

CFD models refer to the numerical (mathematical) models constructed to be solved on computers to represent and investigate settling tanks.

Physical models refers to laboratory bench sized models used to calibrate and test the CFD models.

Mesh; grid

These two terms are also used interchangably in CFD literature to describe or refer to the structure of small cells with which the object or process to be modelled is represented. Both will be used in this document.

1. INTRODUCTION

1.1 Background

Throughout history water has been considered to be a free resource. At least in principle it was also held to be an unlimited one, albeit not necessarily easily available. During the 20th century the reality that this is not the case began to assert itself. This was due to the ever increasing demand reaching the limits of the available supply, the reasons for that being mainly the following:

- Population growth.
- Increased standard of living with concommittant increased usage.
- Increasing industrial and agricultural requirements.
- Pollution and degradation of sources, coupled with overloading of the natural purification mechanisms.

People are becoming increasingly affected by, and therefore also aware of, the fact that water is in reality a finite and valuable resource. Stander (1995:12) calculates the real socio-economic value of water in SA to be an average of R40/m³ in the Gauteng and Western Cape provinces. Due to the change in public perception of water from that of an inexhaustible supply to that of a scarce resource, as well as the increasing real scarcity of water, it is inevitable that the price of water will begin to increase towards the real value. Furthermore, the relative real value itself will also increase. This makes it imperative that more attention should be paid to it than in the past - not only because of general public opinion and legislation, but also for strategic and economic reasons.

The problem of decreasing availability and increasing cost of water can be addressed in a number of ways:

- Forcing consumers to initially waste less and finally use less by means of formal measures like restrictions, fines and tariff increases.
- Rewarding savings achieved.
- Education of the general public.
- Developing and utilizing appropriate water-saving techniques.
- Recovering and rehabilitating damaged sources.

The first order of priority should be to make the best possible use of what is available, i.e. to effect a significant saving in consumption. This can be achieved in the following ways:

- Manage water utilization in an optimum manner, e.g. by use of appropriate watersaving techniques.
- Extend and thereby increase utilization through recycling.
- Preserve the highest possible water quality by preventing pollution, or limiting it if unavoidable. Practise zero-effluent recycle operation.

In reuse and recycling an important component is wastewater treatment. Apart from the fact that recycled wastewater is an obvious water "source", recycling will prevent pollution of other sources. Legal requirements already enforce stringent limits, e.g. the 1 mg/l P limit on municipal wastewater. This in turn requires treatment to a very high quality before release in the natural water cycle, often making it viable to recycle. However, whether recycled or released to an existing water body, the water must be treated.

As stated earlier, release of untreated or inadequately treated water in the "natural" environment causes pollution and degradation of water sources. This has the following ramifications:

- Direct detrimental effects on health of consumers due to ingestion of pathogens, heavy metals and toxic substances.
- Destruction of the natural environment and its aesthetic aspects, which amongst others leads to financial losses due to reduced value of waterfront properties.
- Reduction in the possible uses of the water resource.
- Increased mineralization also causes increased corrosion of water conduits, treatment plant and household appliances, leading to considerable financial losses.
- A major impact due to pollution is eutrophication of water bodies, especially in tropical climates such as in South Africa.

Water treatment processes also impact on water quality. In order to minimise these impacts, it is necessary to operate treatment plants in an optimum manner. For this purpose a thorough theoretical understanding of the processes, as well as the necessary tools and techniques for their operation is required.

Sedimentation tanks are the workhorses of any water purification process. It is thus crucial for the sedimentation tank to be operated to its full potential. It is not only the chemical aspects of flocculation that cause problems, however. Hydraulics also play a prominent part. Overdesign of plant is common, leading not only to unneceassary capital expenditure, but also to water wastage in the form of excessive sludge. Inadequate design causes overloading of filters, leading to frequent backwashing which also wastes a significant percentage of treated water. Many plants are already a few decades old and do not incorporate the latest developments in technique, e.g. inlet and outlet design. Sedimentation tank performance is strongly influenced by hydrodynamic and physical effects such as density driven flow, gravity sedimentation, flocculation and thickening. In turn the velocity and density patterns in tanks influence these processes and are therefore of great interest to design engineers. For older plants the characteristics of the solids that has to be removed have also changed since the original design, e.g. due to eutrophication.

The models that are available for the sedimentation process range from empirical models which are based on an oversimplification of the hydraulics of clarifiers, to more complex numerical models that are based on fundamental fluid mechanics. Availability of an efficient model will lead to a better understanding of the sedimentation process and will make it possible to simulate the effects of design and geometric changes made to a tank. This will lead to two benefits:

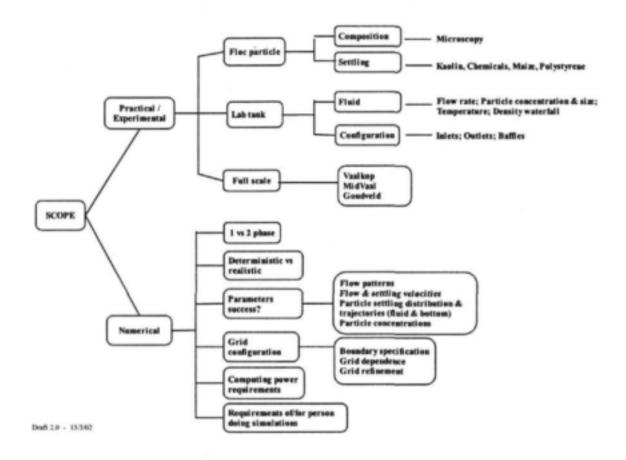
- Improved design of new tanks, leading to fewer failures, or less overdesign to achieve the required capacity, which means capital savings.
- b) The ability to confidently retrofit existing tanks which are currently underperforming or overloaded with simple solutions, thus avoiding the need for expensive extensions.

1.2 Research objectives

The main aim of this project was to demonstrate and gain a better understanding of the processes which influence the operation of sedimentation tanks. The second objective is then to provide design engineers with guidelines and tools to enable them to design cost-effective sedimentation tanks. The third objective is to provide operators of sedimentation tanks with tools which can be incorporated into control systems for the proper operation of these installations. The fourth objective is to evaluate the suitability of CFD for simulations for design of and research into sedimentation tanks.

The study focused on the use of numerical modelling using computational fluid dynamics (CFD) as a tool to enhance the understanding of the operation of sedimentation tanks. The aim was to (i) develop realistic models; (ii) demonstrate the accuracy of the numerical models; (iii) improve the understanding of the physical processes. This understanding will be beneficial to the water industry at large, which includes a wide spectrum of role players from design engineers to operators and for potable water treatment as well as sewage treatment plants. It was carried out by means of research and development work in the following categories:

- Design of numerical models of sedimentation tanks based on the commercial numerical code Flo++ and validation of the models with laboratory experiments and comparison with full scale sedimentation tanks.
- CFD modelling of the influence of manipulating design and operational tank parameters.
 - Design parameters: tank dimensions, inlet and overflow configurations and baffle placement.
 - Operational parameters: flow rate, particle size and concentration, density effects, water temperature, wind.



2. SETTLING AND SEDIMENTATION TANKS

2.1 Sedimentation tanks in water treatment.

In order to appreciate the importance of optimization of sedimentation tank performance, it is necessary to consider the functions of these tanks in water treatment.

2.1.1 Substances removed by sedimentation process.

The type, composition and relative concentrations of the solid material suspended in raw water sources varies widely over space and over time (seasons) at a location, but the following generic classification applies:

- Mineral (clay) particles (silicates).
- Insoluble salts e.g. Fe(OH)₃, MnO₂, metal sulphides, asbestos fibres, CaCO₃ and Mg(OH)₂.
- Micro-organisms: Viruses, bacteria, protozoa, algae and diatoms.
- Organic material: These originate mostly as decay products from dead organisms or are shed by living ones (e.g. leaves from trees). It includes macromolecules and polymers such as humic and fulvic acids, proteins and fibres (e.g. cellulose).

2.1.2 Functions of sedimentation tanks in water treatment.

The primary function of sedimentation tanks is to remove the abovementioned solids. This reduces turbidity and colour, which improve the aesthetic quality. It also reduces the load on filters. However, in doing this the tanks also serve important secondary functions. Because they remove micro-organisms, they aid in the disinfection process. As an added bonus this reduces Cl₂-demand, which reduces costs and helps to produce less THMs, which is both an aesthetic problem and a health risk in water that has been highly eutrophied. This is because THMs are carcinogenic and also an aesthetic problem, since it imparts a smell and taste to water.

The action of the tanks balance seasonal and long-term variations in water quality, i.e. provide water of standard, homogeneous quality to consumers over time. To a lesser extent they also balance water supply and quality from different sources.

2.1.3 Consequences of poor sedimentation tank performance.

The most prominent effect is the increased load on filters, leading to longer filter down-time for backwashing and maintenance. This increases costs and reduces plant capacity. The sand filter is necessary because some algae and bacteria do not flocculate well, and are not removed in the settling tank. To clean the sand filter, the filter is backwashed by blowing compressed air and clean water from beneath the filter bed. During backwashing the sand is ground finer, the air supply system is eroded and a lot of energy is consumed. The water used to clean the filter is also lost, unless it is recycled. Should the settling tank be inefficient, the sand filter loading increases and so too do the detrimental effects.

As an example, a settling tank could remove 97% of incoming solids under favourable conditions. Should conditions change and removal efficiency drop with 3% to 94%, the filter loading doubles from 3% to 6% of tank loading. This causes the filter cycle time to be halved, and thus backwashing frequency to be doubled. The energy consumption of the purification plant is therefore highly dependent on settling tank efficiency.

A second effect is reduced water quality because of higher turbidity and higher pathogen population. This causes health risks and higher Cl₂ demand which in turn causes higher THM concentration.

Lower solids concentration in the sludge produced means water and energy wastage and bigger sludge disposal costs. The volume of sludge removed from the settling tank constitutes a loss; 1 to 4 percent of the inflow to a settling tank is lost as sludge outflow (Pietersen, 2002; Van der Walt, 2000) Inefficient flocculation and settling decreases the solids content and increases water loss as part of the sludge. Very often plant operators try to rectify the problem by increasing coagulant dosages. This increases costs (for chemicals, dosing equipment and longer flocculation channels). It might also require flocculant aids. Increased chemical dosage also means that water quality deteriorates.

Capital expenses are incurred due to modifications or retrofitting in order to bring performance up to the required level. The plant may also require more "hands-on" (as opposed to automated and standardized) operation, which means increased manpower requirements (in terms of number of people as well as their level of training) and more strenuous operation.

Lastly, with overdesigned tanks with too long retention times, there is a problem with secondary algal growth and fermentation with the associated taste and odour imparted to the water and operational problems involved in removing fermented material from the tanks. This was illustrated by one of the authors' experience at the Von Bach purification works at Okahandja, Namibia, that supplies water to the central region of Namibia. Secondary algal growth and algal fermentation caused very high chlorine demand, as well as taste and odour problems.

2.1.4 Rectangular sedimentation tanks

In sedimentation tanks the solids concentration must be increased from the inlet concentration to the concentration of the sludge in the underflow outlet. In the preparation of potable water, virtually all of the solids requiring removal are heavier than water: therefore sedimentation with gravity as the driving force is the most common separation technique, although separation may occur by flotation if the water is denser than the solid matter (Peavy et al, 1985).

Criteria for the design of settling tanks have evolved as much from practice as from theory. Settling tanks employed for solids removal on water-treatment plants are classified as long-rectangular, circular, or solids-contact clarifiers. In this project only long-rectangular tanks were considered.

Rectangular tanks are commonly used in treatment plants processing large flows. The bottom is slightly sloped to facilitate sludge scraping. A slow-moving mechanical sludge scraper continuously pulls the settled material into a sludge hopper where it is pumped out periodically. A schematic representation of a typical rectangular tank is shown in Figure 2.1:

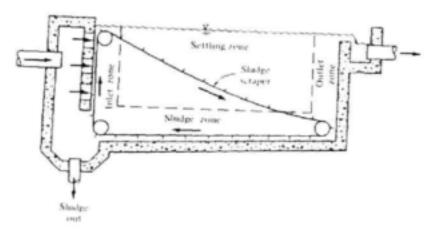


Figure 2.1 Schematic view of rectangular sedimentation tank (Peavy et al, 1985:124).

Figure 2.1 shows that a rectangular settling tank can be divided into four different functional zones:

- The inlet zone designed to spread the flow uniformly both horizontally and vertically across the tank, often by means of baffles.
- The outlet zone in which water flows upward and over the outlet weir.
- The sludge zone, which extends from the bottom of the tank to just above the scraper mechanism.
- The settling zone, which occupies the remaining volume of the tank (Peavy et al, 1985: 123-124).

2.2 Characterization of floc particles

2.2.1 Characterization of floccules in settling tanks

In Southern Africa raw water sources tend to be eutrophic (at least periodically) due to climatic conditions. Directly after rainfall, which occurs as thunderstorms over most of the region, the silt content of surface water increases, especially the mineral part. After periods without rain sunlight stimulates algal growth. Thermal inversion of reservoirs at seasonal changes also occur, which causes algal blooms. The composition of turbidity in the water therefore varies over time, with differences in the organic and mineral fractions.

The mineral particles generally have a higher density than micro-organisms (typically > 2 kg/dm³ compared to just slightly higher than 1 kg/dm³). Also, micro-organisms (especially algae) have all sorts of mechanisms to enable them to not settle out but instead maintain an optimum depth e.g. for photosynthesis (Pieterse & Cloot, 1997). Mineral particles of much smaller size than algal cells will therefore settle gravitationally.

When turbidity is coagulated and flocculated, the formed floc differs from the original particles in density, size and shape. Metal hydroxides generally form "soft" gelatinous flocs containing water in their structure. The settling characteristics of the flocs can therefore not be inferred from the characteristics of the original particles.

This raises the following issues which have bearing on the modelling of settling particles in sedimentation tanks:

1. The extent of organism-mineral mixing in flocs.

To what extent does the formed flocs contain mixtures of organic and mineral components? Or do the organic and inorganic materials tend to agglommerate in separate floccules? This should depend on physical aspects such as the surface charge (zeta potential) of the respective particles and, probably, the interaction between the particles and the coagulant used in a particular case.

This aspect can be researched by means of microscopy and X-ray analysis on a SEM. Preliminary work by means of optical microscopy was done during this project using water from the Mooi river in Potchefstroom with metal (Fe, Al and Ca) hydroxides as flocculants. It showed that the flocs were composed of mixtures of all the solid material in the water, *i.e.* clay, fibres, algae, bacteria and diatoms. Cornelissen *et al* (1997) also report on work in this regard.

2. The actual or realistic density of flocs in water for modelling.

This bears directly on the previous point. The real density of the floc in the water will normally not be a weighted average of that of its turbidity constituents, due to the reasons given above. An obvious complication is the presence of captive water molecules in the floc structure of hydroxide flocs. Also there are some other practical questions, e.g. what is the real "dry" density of algal particles? Does that refer to the normal, living algal cells out of the water, or to desiccated cells? In fact, the water content of the gelatinous metal hydroxide flocs causes the same uncertainty.

3. The effective size and shape of flocs.

The available models normally assume homogeneous and spherical particles. This is not the case in reality. However, it is likely that a particular floc will display constant features, e.g. fractal dimension, which can be utilised in characterising it and modelling its settling behaviour. It will be necessary to determine the typical structures, shapes and sizes of flocs consisting of various turbidity components formed by using various different flocculants.

Characterization methods to obtain the abovementioned information.

This also follows directly from the previous point. It is necessary to find methods of characterising the physical properties that determine the settling behaviour of the flocs in a quantitative manner. These methods need to be simple and quick in order to be of use in water treatment plant operation. For design purposes more sophisticated methods can be used, e.g. zeta potential measurements, particle counting and SEM analysis.

5. What is the (realistic) size distribution and composition of turbidity components in surface waters in Southern Africa to be used as parameters in design of full-scale plant and for modelling purposes?

This is the basic question underlying the above analysis. It was found to be such a large issue that it justifies a project of its own.

2.2.2 Mathematical description of particle settling

Sedimentation may be classified into various types depending on the characteristics and concentrations of suspended materials (Peavy et al., 1985 : 114).

Particles whose size, shape and specific gravity do not change with time are referred to as discrete particles.

- Particles whose surface properties are such that they aggregate, or coalesce, with other particles upon contact, thus changing size, shape and perhaps specific gravity with each contact, are called *flocculating* particles.
- Suspensions in which the concentration of particles is not sufficient to cause significant displacement of water as they settle or in which particles will not be close enough for velocity field interference to occur are termed dilute suspensions.
- Suspensions in which the concentration of particles is too great to meet these conditions are termed concentrated suspensions. (They are mostly found in wastewater treatment.)

These differences result in significantly different settling patterns and require separate analysis.

Other authors make similar distinctions and classifications. (Takacs et al, 1991), state that, depending on the nature and concentration of the solid particles, four types of settling characteristics are normally encountered in <u>wastewater</u> treatment plants:

- Discrete particle settling. Associated with the removal of grit and sand particles, discrete particle settling is characterized by solids which settle as individual entities with little or no interaction with other particles.
- Flocculant particle settling. Typical of the type of settling found in primary clarifiers, and the upper layers of a secondary settler, flocculant particle settling is characterized by the flocculation of solid particles as they settle through the water column.
- Hindered settling. Suspension in which inter-particle forces hinder the settling process. The mass of particles settles as a unit.
- Compression settling. "Settling" is achieved by compression of the mass of particles. Compression results from the weight of particles added to the system.

Type-1 settling (discrete particles in dilute suspensions) is the type of settling encountered in the settling zones of rectangular sedimentation tanks in purification plants for potable water treatment in South Africa, because:

- 3. Particle concentrations in the raw water from surface streams and dams are low.
- There is a very large particle size distribution.

There are very diverse (inhomogeneous) physical particle types (in terms of shape, density and surface charge).

In contrast, in wastewater treatment, especially sewage water treatment, the flocs produced by biological treatment processes have much higher concentrations (typically in the hundreds of mg/l) and much more homogeneous composition i.r.o. size, shape and density. Therefore it exhibits zone settling.

Type-1 settling

Discrete particles in dilute suspension undergo Type-1 settling. This case is the easiest to analyze (Peavy et al, 1985: 114) If a particle is suspended in water, it has two forces acting on it:

The force of gravity

$$F_g = \rho_g g V_p \qquad (2-1)$$

With: ρ_k the density of the particle g = gravitational constant $V_p = \text{volume of particle}$

The buoyant force (quantified by Archimedes)

$$f_b = \rho_n g V_p \qquad (2-2)$$

with: ρ_{κ} = density of the water

If the density of the particle differs from that of the water, a net force is exerted and the particle is accelerated in the direction of the force:

$$f_{net} = (\rho_p - \rho_n)gV_p \qquad (2-3)$$

Once motion has been initiated, a third force is created due to viscous friction, called the drag force:

$$f_d = C_D A_p \rho_\kappa \frac{v^2}{2} \qquad (2-4)$$

where C_D = coefficient of drag

 A_p = cross-sectional area of the particle perpendicular to the direction of movement

v = velocity of particle

The drag force acts in the opposite direction to the driving force and increase as the square of velocity, therefore acceleration rate decreases until a steady velocity is reached at the point where the drag force equals the driving force:

$$(\rho_p - \rho_n)gV_p = C_D A_p \rho_w \frac{v^2}{2}$$
(2-5)

For spherical particles of diameter d,

$$\frac{V_p}{A_p} = \frac{\frac{4}{3}\pi(d/2)^3}{\pi(d/2)^2} = \frac{2}{3}d$$
(2-6)

Substituting into equation (1-6) gives for the terminal settling velocity v_r of a sphere in water

$$v_z^2 = \frac{4}{3} g \frac{(\rho_p - \rho_w)d}{C_D \rho_w}$$
(2-7)

For laminar, transitional and turbulent flow the values of C_D are:

$$C_D = \frac{24}{\text{Re}}$$
 (laminar) (2-8)

$$= \frac{24}{Re} + \frac{3}{Re^{1/2}} + 0.34 \quad \text{(transitional)}$$
 (2-9)

where Re is the Reynolds number

$$Re = \frac{\phi v_s \rho_w d}{\mu}$$
 (2-11)

For laminar flow, substitution of Eq. (1-8) into Eq. (1-7) yields:

$$v_x = \frac{g(\rho_p - \rho_w)d^2}{18\mu}$$
 (2-12)

which is known as the Stokes equation.

To summarize: The Stokes equation gives the terminal settling velocity of a spherical particle with laminar flow around it. This is obviously not realistic for real flocs, but can be used as a first approximation to give an upper boundary value for particles of a given diameter and density.

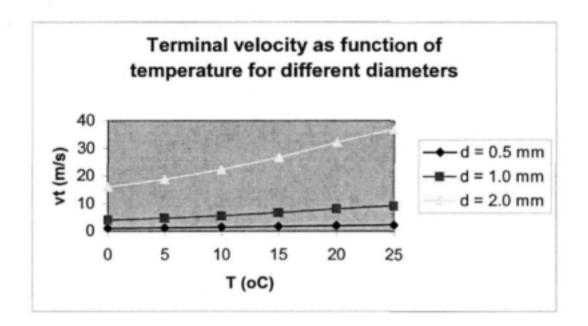
It must be noted that the buoyant force is much more important in CFD models for sedimentation tanks than for the original aerodynamical applications for which CFD was developed. CFD packages generally make provision for modelling particles in the fluid. However, originally these typically were dust or soot particles in heated gasses. In these applications, the weight and drag forces were very much larger than the buoyant forces because the density of the particles is very much larger than that of the gasses. The buoyant force was therefore ignored to simplify calculation and reduce computation time. This did not create any significant error or inaccuracy for such applications. In the case of floc particles in water, the density of the particles is very close to that of the water and the buoyant force becomes very significant, almost balancing the weight. It must therefore be included in the numerical description of the system. In the Flo++ package used to develop the models this was done by means of the user-coding facility provided.

Thickening.

A number of authors provide overviews and cover the development of equations to describe or model settling of solids at higher concentrations (thickening). Recommended is the publications by Takacs et al (1991), Hill (1985), Dick and Ewing (1967), Vesilind (1968), Keinath et al (1977), Patry and Takács (1991) and Roth and Pinnow (1981). Since the operating conditions for these were not applicable to this study, it is not expounded further. It would however be an obvious further step in the development of the work reported on here.

The effect of water temperature on settling rate.

Both the density and the viscosity of water change with change in water temperature. Appendix C gives the details of these changes. A change in density will affect the relative weight of the particles and a change in viscosity the drag force on the particles. Since both density and viscosity of water decrease with temperature, the particles will settle out more rapidly at higher temperature, as can also be seen from the Stokes equation. This effect is shown in graph 2.1.



Graph 2.1 The effect of water temperature on particle settling rate.

The density of the particles in the calculations were taken as 1013,031, since this was the density of the crystalline polystyrene used as the floc simulant during the physical experiments. The equations used to calculate the forces and settling velocity were

$$v_t = \frac{g(\rho_p - \rho_w)d^2}{18\mu}$$
 (the Stokes equation)

and

$$f_d = \frac{4}{3}\pi \left(\frac{d}{2}\right)^3 \left(\rho_p - \rho_w\right)g$$

2.2.3 Numerical description of particles.

The structure of floc particles that is very irregular cannot be fully described numerically as either two or three dimensional objects. To describe such structures, fractal geometry is used nowadays (Addison, 1997). This is a relatively new field of mathematics that is still undergoing rapid development, but has been applied to the study and description of floc structure, e.g. by Logan & Kelps (1995). They used fluorescent carboxylate microspheres (type YG, Polysciences Inc.). The fractal dimensions of aggregates produced in a rolling cylinder was determined as $D_3(l,v) = 1.59+-0.16$, while aggregates produced in a paddle mixer had a higher fractal dimension of $D_3(l,v) = 1.92+-0.04$. These experiments demonstrated that aggregate properties are a function of the fluid mechanical environment used to coagulate particles.

Cornelissen et al (1997) studied hydrous floc precipitates of aluminium and iron. In their work they also investigated the effect of pH on structure and found that their results correlated well with experiments by Botero et al (1991), who found that an increase in pH corresponds to an increase in fractal dimension and therefore with an increase in the density of the precipitate.

Nakamura et al (1993) determined the fractal dimension of single Microcystis colonies from dense surface blooms in Lake Kasumigaura as 2.5. They refer to the work of Tambo and Watanabe (1967, 1979) who measured the settling velocity of kaolinite floc as a function of floc diameter. The latter found that the density of floc decreases with an increase in floc diameter in accordance with a power law. This power law implies that the floc has a fractal structure which is usually described by

$$i = \left(\frac{D_f}{d_o}\right)^D$$

In adapting this work to describe the settling of *Microcystis* flocs Nakamura and his colleagues combined the above equation with Stokes' law to derive the following equation for the vertical movement:

$$V_f = \frac{g}{18\mu} \Delta \rho d_o^2 \left(\frac{D_f}{d_o}\right)^{(D-1)}$$

where

do = diameter of a spherical domain occupied by a single cell which is surrounded by a slime layer.

D = fractal dimension

 D_r = diameter of a floc

g = acceleration due to gravity

i = number of cells (or the domains) contained in a floc

 V_f = terminal flotation velocity of a single floc

 μ = viscosity of surrounding liquid

 $\Delta \rho$ = effective density of the cell domain (= $\rho_v - \rho_0$)

In the derivation it is assumed that each colony is a spherical floc which has a fractal structure, pores in the floc are filled with surrounding liquid and liquid flow through the moving floc is negligible. These were also the assumptions used for the models in this project.

Chen (1998) used suspensions of negatively charged kaolin clay flocculated with nonionic, cationic and anionic polyelectrolytes as a model system for the orthokinetic flocculation process. According to Chen both cylinder tests and jar tests using low shear conditions tend to underestimate the polymer dosage requirements for the orthokinetic flocculation process. Under prolonged shear conditions, optimum polymer dosages required for maximum turbidity removal or minimum residual turbidity coincide with those required for zero zeta potential or plateau adsorption of polymer.

2.3 Design of rectangular settling tanks

2.3.1 Conventional approach and guidelines for design

The conventional approach to the design of rectangular sedimentation tanks is described in the standard water engineering handbooks, of which Peavy et al (1985) and Metcalf & Eddy (Tchobanoglous & Burton, 1991) are typical examples. The procedure entails the following steps:

- The terminal settling velocities and size distribution of the typical floc particles that are to be removed in the tank are determined with settling tests. With the help of settling column analysis the settling velocity of the particles is measured. With this settling velocity the overflow rate of the tank is defined. The depth of the tank is chosen and used for the settling column analysis. The settling column has the same height as the tank.
- These parameters are then employed to calculate an overflow rate (m³/m².h) that will provide adequate solids removal in the settling zone of the tank.
- From the obtained settling tank overflow rate and raw water flow rate, the tank is then sized and inflow and outlet weirs designed.

The required capacity of the purification works is used as the main design parameter. With the volume flow rate and the overflow rate the surface area is calculated as $Q = q_0 A_0$

A length-to-width ratio is chosen (mostly 3/1) and the surface dimensions are calculated

$$w \cdot 3w = A_s$$

$$(3.2)$$

The retention time is established by

$$t = \frac{V}{Q \frac{1}{24}}$$
(3.3)

The horizontal velocity is calculated by

$$v_k = \frac{Q}{24A_s}$$
(3.4)

The overflow length will be the width or a multiple width of the tank. The designer chooses this length. The weir overflow rate is than calculated by

$$\frac{1}{24}Q \bullet \frac{1}{I_O} = \text{overflow rate}$$
(3.5)

Inlet and outlet zones are added, sized relative to the depth of the tank, as well as a sludge zone as shown in the example in Figure 2.2.

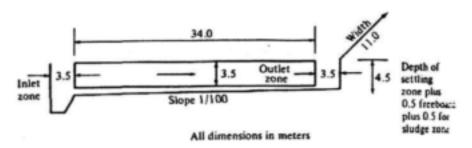


Figure 2.2 Design example for inlet-, outlet- and sludge zones (Peavy et al, 1985).

In this method of design the particles are assumed to settle in a straight line as shown in Figure 2.3. The vertical velocity measured in the settling column and the horizontal velocity from the inlet are used to calculate the absolute velocity, and thus trajectory, of the particles.

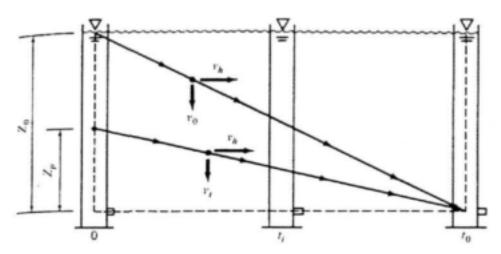


Figure 2.3 Settling path and velocity vectors of particles according to conventional design method (Peavy et al 1985).

The calculations are generally based on density and dynamic viscosity values for water at 20 °C. For these calculations, the floc density is also normally taken as being of the order of 2 to 3 kg.dm⁻³, as is typical for floc containing predominantly mineral (clay), rather than organic (especially algal) material. The calculations are also based on the following explicit and implicit assumptions:

 Water flow through the settling zone is uniform and not affected by the settling particles. The particles' settling trajectories can therefore be considered as linear

- for discrete flocs, and as parabolic for coagulating flocs. The settling characteristics of the floc particles as determined by the settling cylinder tests can therefore be applied directly to the design of the tank (Peavy et al, 1985).
- The characteristics of the suspended solids, and thus the flocs formed, do not change significantly over time. I.e. floc size, shape, density and settling rate remains fairly constant over the operational life for which the tank is designed.
- The effect of temperature changes in the raw water on the hydraulics of the tank, and therefore on floc settling, is negligible.

2.3.2 Limitations of the conventional design approach

All three of the abovementioned assumptions are invalid in practice. Van der Walt (1994) and Du Toit and Lemmer (2000) has shown that assumption 1 is invalid because the settling particles causes a definite density waterfall at the inlet of the tank, thus completely changing flow patterns and horizontal and vertical velocity profiles in the tank from the idealized uniform situation. On entering the flow plunges almost immediately towards the tank bottom, after which it continues along the tank bottom. The potential energy that exists as a result of the excess density is converted to kinetic energy at the tank bottom that result in a strong bottom current and extends the full length of the tank, slowing down towards the shallow end. The potential energy available in the mixture is reduced as solids settle out of the bottom current, thereby reducing the kinetic energy of the bottom current. Some of the kinetic energy is converted back to potential energy due to resuspension. This is clearly the case close to the inlet where the return current reintroduces solids into the relative clean supernatant. The bottom current is therefore primarily driven by density differences and the pressure gradients play only a secondary role.

To balance the strong bottom current an eddy is formed at the surface. The eddy slows down more rapidly than the bottom current as fluid is withdrawn from the launders at the water surface. (Van der Walt, 1994: 90-91)

In surface water bodies in the tropics, where South Africa is also situated, the second assumption is not valid either because the composition and characteristics of the solids comprising the turbidity in the water is subject to seasonal changes. The relative and absolute concentrations of the respective mineral and organic constituents changes significantly over the course of a year, affecting the sizes, densities and composition of flocs formed after coagulation. When the raining season starts in spring, water in the rivers contains high concentrations of mineral (clay) particles, because land has been denuded by harvesting and grazing during winter. In the autumn, the land surface is covered with vegetation. Rainwater draining to rivers is clearer and enriched with fertilizer from fields. This causes an increase in especially algal populations. Consequently in spring turbidity will therefore tend to form flocs with a higher relative mineral content and therefore greater particle density than in autumn.

Surface water temperatures on the highveld of South Africa vary significantly during the course of a year. In Potchefstroom the temperature of water from the tap as recorded during the experiments reported on here varied between 11 and 26 °C during the course of 10 months which included summer, autumn and winter seasonal changes. Similar variation was observed over the past six years. Data obtained from the Department of Water Affairs and Forestry for the Vaal river at the Barrage for the period from January 1998 to December 2000, gave a lowest temperature of 8,5 °C and a highest of 25 °C. Typical variations between winter and summer were from 11 to 22 °C. The temperatures at the Barrage and at Midvaal Water's plant at Orkney correlated well. The temperatures tended to change from high to low within only a few days with the advent of cold fronts, and also increased quickly with warmer water. The changes were normally not gradual. The temperature changes affect both the density and viscosity of the water, which has an effect on the hydrodynamics of water flow and particle settling.

Water temperature also affects the rate of coagulation and flocculation. The velocity gradient G is considered a key parameter in flocculation kinetics. G is dependent on the viscosity (Elmaleh and Jabbouri, 1991).

3. COMPUTATIONAL FLUID DYNAMICS (CFD)

3.1 CFD Modelling

The advantage of CFD is that the actual flow in the tank can be simulated. For example: Figure 3.1 shows the actual flow in the tank by means of vectors. It can be seen that the particles do not settle in a straight line, but that there is a density current, or "waterfall", at the inlet. The traditional model assumes that the particles do not affect the flow of the water. Practical experience has shown that this is incorrect and CFD studies confirmed it. A far more optimised design can be made if CFD analysis is done because the effects of any modification to the tank can be made visible.

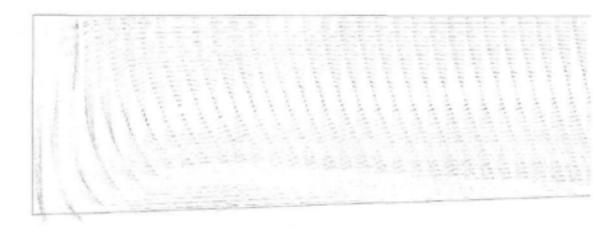


Figure 3.1 Vector plot of the flow in a sedimentation tank modelled with Flo++

The first sedimentation tank designed with CFD has been built for an extension of the Vaalkop purification works in South Africa during the year 2000. The first results show an improved product water quality in comparison to the existing tanks.

3.1.1 Basic methodology of CFD

Computational Fluid Dynamics (CFD) can be described as the use of computers to produce information about the ways in which fluids flow in given situations. CFD embraces a variety of sciences including mathematics, computer science, engineering and physics, and these disciplines have to be brought together to provide the means of modelling fluid flows. (Shaw, 1992)

There are several approaches to doing this. In this project the finite volume method was used. This is done basically by means of the following procedure:

- The physical configuration of the body in which the flow takes place is described mathematically.
- This mathematical description consists of breaking up the body in a very large number (thousands to millions) of small cells (volumes), called a grid or mesh.
- The behaviour of the liquid in each of the cells in the grid is determined by the relevant laws of physics, i.e. the laws of conservation of mass, momentum and energy and the laws of motion.
- These laws are written in a form that can be solved iteratively as a set of numerical equations on a computer for the fluid or fluids and particles in each cell.
- To solve such a set of numerical equations, the initial conditions (including volume or mass flow rate, temperature, viscosity, density, pressure and concentrations or fractions) have to be specified.

To obtain an approximate solution numerically, we have to use a discretization method that approximates the differential equations describing the physics by a system of algebraic equations, which can then be solved on a computer. The approximations are applied to small domains in space and/or time so that the numerical solutions provide results at discrete locations in space and time. Much of the accuracy of experimental data depends on the quality of the tools used, e.g. the accuracy of numerical solutions is dependent on the quality of discretizations used. (Versteeg and Malasekera, 1995.)

Computational Fluid Dynamics is not a replacement for the traditional experiments that are used to study the flow patterns in a sedimentation tank. It is rather an additional tool to the traditional methods used to model or describe flow patterns and to design a sedimentation tank.

CFD can be seen as numerical experiments and the advantages of these "experiments" over the traditional experiment-based approaches to fluid system design/simulation are:

- Substantial reduction of lead times and costs of new designs.
- The ability to study systems where controlled experiments are difficult or impossible to perform (e.g. very large systems).
- The ability to study systems under hazardous conditions at and beyond their normal performance limits (e.g. safety studies and accident scenarios).
- 4. Practically unlimited level of detail of results.
- 5. Testing of design and operation concepts before implementation.

The variable cost of a physical experiment, in terms of facility hire or man-hour costs, is proportional to the number of data points and the number of configurations tested. In contrast CFD codes can produce extremely large volumes of results at virtually no added expense and it is very cheap to perform parametric studies, for instance to optimise equipment performance. In the water industry modelling using CFD has not been widespread because of the associated costs, lack of powerful enough computers needed for complex problems and unfamiliarity with the mathematical models. This situation is changing at present because of the increase in computer power with decrease in costs.

The theory of CFD is mathematically advanced and requires background knowledge of physics, numerical analysis and computer programming beyond the scope of this report, therefore it will not be presented here. What follows is a generic description of the steps and processes involved.

CFD codes are structured around the numerical algorithms that can tackle fluid flow problems. In order to provide easy access to their solving power all commercial CFD packages include sophisticated user interfaces to input problem parameters and to examine the results. All codes contain three main elements as shown in figure 3.2.

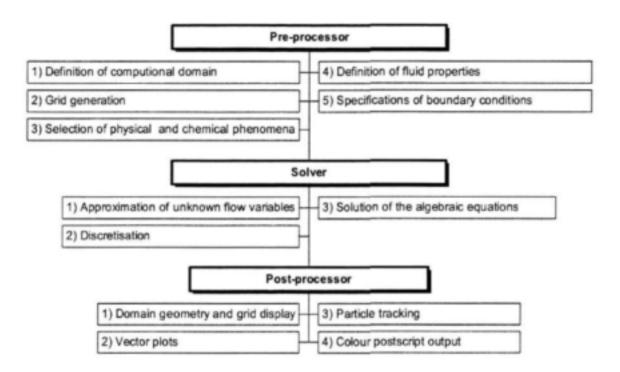


Figure 3.2 Structure of CFD packages.

The solution of the algebraic equations is done by an algorithm shown in figure 3.3.

A general understanding of the diagram is sufficient, because the computer code of the commercial packages (e.g. Flo⁺⁺ as used in this project) contains the equations and solves them. Total understanding of the discretization of the equations would require a course in CFD.

The results generated by a CFD code are at best as good as the physics embedded in it and at worst as good as its operator. A good solution must be consistent, must converge and must be stable as the grid spacing is reduced to zero. (Versteeg and Malalasekera, 1995)

Partial differential equations are used to describe viscous turbulent flow. Conservation of mass (continuity) and conservation of momentum is the basis of these equations. In order to solve these equations, the flow domain is discretized, or divided into cells (control volumes). The accuracy of the solution is dependant on the number of cells used to discretize the domain.

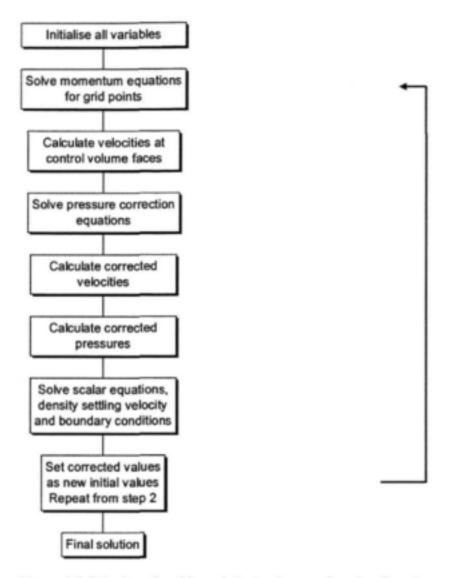


Figure 3.3 Solution algorithm of algebraic equations by the solver

The SIMPLE algorithm presented by Patankar (1980) is used to solve the 3-D continuity and momentum equations. This algorithm is developed by using the finite control volume method with the variables for velocity {U, V, W} and pressure p computed on a co-located grid; i.e. the values of pressure and U, V and W are calculated at the cell centre. The partial differential equations are discretized on a non-uniform computational grid.

The resulting algebraic equations are solved using a line-by-line iteration. The number of iterations to reach a converged solution depends on the densimetric Froude number Fd, the grid distribution, and the aspect ratio (length to width) of the tank. McCorquodale and Zhou (1993) have found that density flows (such as found in

sedimentation tanks because of the presence of the floc particles and settled sludge) typically require a computation time an order of magnitude longer than neutral density flows. (McCorquodale 1997)

Physically unrealistic property gradients caused by the numerical method is called numerical diffusion. Numerical diffusion depends on the accuracy and the type of differencing scheme used as well as the grid distribution and orientation with respect to the velocity vector. It has been shown that neutral density flows experience more diffusive errors than the density flows. (McCorquodale 1997)

The simplest discretization scheme is the first-order UPWIND scheme. A second order scheme (limiting numerical diffusion) is the QUICK scheme (Leonard 1979). The QUICK scheme is computationally more costly than the UPWIND scheme. Where sharp gradients are of importance to the solution, a higher order differencing scheme can be used, together with appropriate grid refinement.

McCorquodale (1997) recommends that grid dependence be checked by using at least three different grid densities. Grid convergence is indicated if the differences in the flow patterns diminish as the grid refinement is increased. He and his co-workers found mesh sizes in the range 12 x 24 to 24 x 42 (with nonuniform spacing) to be adequate for 2-D modelling of rectangular settling tanks.

McCorquodale (1997) reports that when more sophisticated second- or third order convection discretization schemes such as QUICK and distorted grids were applied, the grid dependence was found to be much more sensitive. Grids in the range of 100 x 150 cells or even finer were necessary to produce grid independent results.

The equations used by Van der Walt (1994) to model momentum, turbulence and solids transport was also used in this study. According to Van der Walt (1994) the process consists of solid and liquid phases which influence each other significantly. To simulate this two-phase behaviour a pseudo Euler/Euler approach is used (see paragraph 3.1.2). A vector equation is solved for the momentum equations and a scalar equation for the solids transport equations. The mixture is taken as a continuum.

3.1.2 Modelling of two-phase systems

There are two approaches available to modelling the flow of water with floc particles in it (i.e. two phases) in a settling tank, viz the pseudo Euler-Euler (scalar) method and the Euler-Lagrange (discrete particle) method.

Pseudo Euler - Euler method (two fluids)

The particles are not modelled individually, but rather as an additional "mixed liquid phase" with properties determined by the calculated values of the mixture components in each cell. The density of the fluid in a given cell is thus a weighted average of the densities of the liquid and the particles (via the concentration) in the cell. This is done by making use of user-coding incorporating <u>scalars</u> into the model. Aspects such as the floc density, settling velocity and concentration are then solved as scalars for each cell in the domain.

Disadvantages and limitations:

- For each different type, size, settling velocity or density of particle a new set of scalars have to be defined, and then solved for every cell in the domain.
 Computational loads very soon becomes excessive if a variety of sludge components have to be incorporated (if their respective properties cannot be incorporated in single averaged values).
- It is therefore also impossible to fine-tune attributes such as particle shape in this type of model.

Advantages:

- For homogeneous flocs (which can be described by a single set of scalars) the model solves much more rapidly than the discrete Lagrangian one which has to track every particle.
- It is (in principle) easier to calculate solids concentrations for every cell in the domain using this type of model.

[Note: This method can also be used to simulate a liquid, coloured tracer injected into the fluid as was done during the experimental simulations in this project. The tracer is modelled as a scalar with the same properties as the water, but displayed in a different colour.]

Euler-Lagrange method (Discrete particles in fluid)

The floc particles are modelled as discrete particles which settle discretely. The solver keeps track of each particle. (In practice the particles are usually combined in "parcels" of particles, to keep calculation requirements manageable.)

In Flo++ three particle tracking modelling options are available:

- No interphase transfer (massless particles).
- Interphase transfer from continuous to dispersed phases (known as uncoupled approach).
- Interphase transfer between continuous and disperse phases (coupled approach).

Limitations and disadvantages:

- The fractional mass and volume of the particles must be small compared to that of the fluid and remain so, even if the particles settle to form a sludge.
- There is no interaction between the particles.
- The solver must keep track of each individual particle in the whole domain, thus either detail is lost by limiting the number of particles, or the computational load becomes excessive very rapidly.
- Because the solver actually solves for parcels of particles, some inaccuracy in the solution is inherent in the method.
- The particles are considered to be spherical for the calculation of their movement (e.g. drag forces).

Advantages:

- It is easy to discretize a variety of particle size distributions, densities and settling velocities in one model.
- The physical behaviour of the model is easily visualised.
- It will probably be easier to incorporate aspects such as shape factors into the equations.

- The particle tracking equations are only solved for the cells actually containing particles, which decreases computation times.
- The actual trajectories of particles can be visualized, which is especially helpful in design. (It must be noted that this is still limited to discrete, specific sizes of particles.)

Particle tracking

Particle tracking refers to computation of the trajectories of discrete spherical particles through a simulated flow field. In this study, particle tracking is evaluated as an alternative to the scalar transport model for two-phase flow.

As explained by Le Grange (1994) under the assumption that the movement of the particles do not influence the flow pattern, the flow is simulated first, and then particle tracks are computed. A solution obtained in this way is called an *uncoupled* solution. If the fluid and particle momentum equations are solved simultaneously, the solution is termed a *coupled* solution.

Coupled solutions are far more realistic than uncoupled solutions. The downside is that coupled solutions can be extremely expensive numerically, and convergence can be difficult to obtain. For the abovementioned reasons, momentum-coupled flow/particle tracking have not been used extensively to model settling tanks.

Stovin and Saul (1998) investigated the settling of solids in sewer storage chambers by using uncoupled particle tracking with FLUENT CFD software. They investigated effects of certain parameters on solids removal efficiency, namely particle density and start location, boundary conditions, number of particle time steps and particle step length factor. Numerical results were compared with experimental results.

Numerical simulation

Flo++ computational fluid dynamics software (version 2.3094 at first and 3.07 later) was used in this investigation. Le Grange developed Flo++ during the 1990's in Potchefstroom, South Africa. Flo++ is based on the finite volume method and uses the SIMPLE algorithm to solve the three-dimensional transport equations.

Handling of particles in Flo++

Flo++ groups particles in "packets" to minimise the computational effort required.

The position of the parcel approximates the position of the centroid of the "cloud" of particles in a cell. The tracks of particles are computed after computing the velocity field. The momentum transfer from a particle to the fluid is treated as a momentum source term in the appropriate cells. Several iterations for solving the flow can be done in between each particle tracking operation. This is referred to as the frequency of tracking.

3.1.3 The densimetric Froude number

For flows involving thermal or concentration-generated density currents, the densimetric Froude number is more important than the standard Froude number related to the free surface gravity waves. The densimetric Froude number Fd is the ratio of the fluid velocity to the internal wave speed at a density interface; or in other terminology, the ratio of momentum to buoyancy or of kinetic energy to potential energy per unit time. For a settling tank inlet it is given as:

$$Fd = \frac{u_{in}}{\sqrt{g'_{in}} H_{in}}$$
with u_{in} : inlet velocity
$$H_{in}$$
: inlet height
$$g'_{in} = g \frac{\rho_{in} - \rho_{in}}{\rho_{in}} = g \frac{\Delta \rho_{in}}{\rho_{in}}$$
and
$$\Delta \rho_{in} = C_{in} \frac{\rho_{p} - \rho_{in}}{\rho_{p}}$$

In this research it is reasoned that d_{in} would be used for round inlets to the tank instead of H_{in} , the height of the inflowing stream. It follows that the densimetric Froude number can be computed with the following formula:

$$Fd = \frac{u_{in}}{\sqrt{C_{in}d_{in}g\left(\frac{1}{\rho_w} - \frac{1}{\rho_p}\right)}}$$

According to McCorquodale (1997) the optimal value for the inlet densimetric Froude number is Fd = 1

- For Fd >1, i.e. when the inlet aperture height is smaller than the optimum height, the kinetic energy or the momentum is dominant and produces an inlet wall jet with high velocities from the origin.
- For Fd < 1, i.e. when the inlet aperture height is higher than the optimum height, the potential energy and thus the density effect becomes dominant and forms a pronounced bottom current that is maintained by the conversion of potential energy into kinetic energy

3.1.4 Aspects Affecting Accuracy of CFD Models

With the rapid increase in computing power, the numerical modelling approach has become more and more useful and feasible as a method to investigate problems related to fluids, including design and operation of components of water treatment plants. However, it also follows from the simplified description given above that there are limitations to this method which must be considered when using it. The most important are the following:

- The model is only as good as the physics used to describe it. If the physical description of a fluid system is oversimplified, the model is inherently limited in accuracy.
- The composition of the computational grid can also have a significant effect on the results. In order to obtain the greatest accuracy in the calculated results, the grid must consist of as many and as small cells as possible, but this requires long computational runs and powerful computers. A balance must therefore be found between grid detail and complexity on the one hand, and computational requirements on the other. This can be handled to an extent by refining the grid in volumes of importance and making it coarser in the rest. Because of this it is necessary to test grid dependence of the solutions generated by a model.
- Fluid flow, as part of nature, is infinitely complex. This complexity is being modelled by means of calculations about finite and discrete volumes of fluid on computes. The computers can also only store and calculate any given real number

to finite accuracy. Any value calculated for any physical parameter in that which is being modelled, is therefore only being calculated to an approximate accuracy. This is also an inherent limitation and requires careful design of the calculation algorithms in order to obtain reasonable accuracy and realism of the calculated solution. For example, rounding-off error accumulation due to a poor algorithm can cause an otherwise good model to fail.

3.2 History of application of CFD models to sedimentation tanks

3.2.1 Examples from literature.

Larsen (1977) did the pioneering work in rectangular settling tank modelling. His research was supported by experimental and field measurements, which provided valuable information on the various hydrodynamic processes in settling tanks. He also described a mathematical model for settling tanks.

As described by Van der Walt (1994) finite volume numerical models developed as follows: Celik et al. (1985) used the SIMPLE algorithm to solve the turbulent momentum equations for a neutral density case. Stamou (1989) added a solids transport equation. Adams (1990) concluded that higher order differencing schemes are required to limit numerical diffusion. Stamou (1991) developed a curvature modified k-ε model to improve the accuracy of the turbulence model. Lyn et al. (1992) used more than one solids transport equation, each with a unique settling velocity. They also included a source term in the solids transport equation for shear flocculation. Krebs (1991) used the PHOENICS code to show the qualitative effect of various geometrical changes. He showed that inlet baffles, dividing walls and energy dissipating devices can increase tank efficiency.

Zhou and McCorquodale (1992) solved the turbulent momentum and solids transport equations. They linked it with a settling velocity formulation and a special bottom boundary condition. Results were compared with the experimental work of Larsen (1977). McCorquodale et al. (1993) investigated the effect of hydraulic and solids loading on a sedimentation tank. They concluded that the densimetric Froude number influenced tank efficiency more than the Reynolds number. Dahl et al.(1994) used the PHOENICS code to simulate a laboratory sized secondary settling tank. Comparisons with experimental horizontal velocities and solids concentration showed good agreement.

Frey et al. (1993) used the VEST code to determine the flow pattern in a sedimentation tank as input for the TRAPS code which determined particle tracks. Olsen et al (1994) used the SIMPLE algorithm to simulate flow in a sand trap.

Van der Walt (1994) used the FLO++ code to simulate three-dimensional effects in the Jönköping tank as reported by Larsen (1977). The effect of crosswind over the tank was also investigated. This study used a scalar transport equation to model two-phase flow. Treating some of the solids-liquid interaction implicitly through the settling velocity reduced the number of variables. Van der Walt also used CFD models to design new settling tanks at Vaalkop, South Africa.

As quoted from McCorquodale (1997), McCorquodale and Zhou (1991) used a threedimensional model to make improvements on square settling tanks in Portland, Oregon.

De Cock, Blom and Berlamont (1998) included a flocculation model in their research into sewer storage sedimentation tanks. Fifteen scalar transport equations were used to model the different size classes of flocs. The flocculation was modelled by changing the concentration of a size class according to the calculated turbulence G-value.

De Cock, Vaes, Blom and Berlamont (1998) conducted a study in which they compared numerical model results and experimental scale model results.

3.2.2 The Jönköping tank

The initial modelling during this project was done to simulate the Jönköping tank, which was described by Larsen (1977). The reason for this is that this tank is well studied and described in literature and serves as a benchmark. This was also the reason that Van der Walt (1994) chose it for his study.

The Jönköping tank is a secondary tank, used in an activated sludge process in a plant at Lund, Sweden. It is designed for a nominal residence time of 3,5 hours. The tank has a bottom that slopes from 3,5-m depth at the inlet to 2,5-m at the downstream end. The influent enters the tank through 4 pipes of 150-mm diameter with a 90-degree bend forcing the influent towards the water surface. The clarified liquid overflows through four launders and the sludge is scraped towards the sludge hopper, located below the inlet pipes. A schematic drawing of the tank is shown in Figure 2.3.

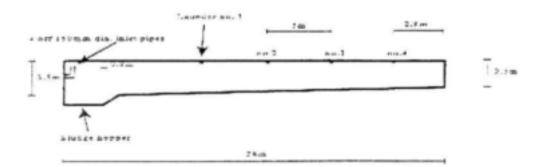


Figure 3.4 Jönköping tank dimensions.

The test conditions that were used are summarised in Table 3.1.

Table 3.1 Jönköping tank test conditions:

Overflow rate	1,7	m ³ /m ² /h
Influent concentration	850	mg/l
Underflow concentration	2400	mg/l
Overflow concentration	± 20	mg/l
Recirculation ratio	0,5	-
Tank length	28	m
Tank width	5	m
Tank depth	2,5 to 3,5	m
Initial settling velocity	4,5	m/h

- The overflow rate is the number of cubic metres that passes through a square metre of the surface per hour. This is the main design parameter.
- The influent concentration is the mass of particles in milligrams per litre that enter the tank.
- The underflow concentration is the mass of particles in the sludge blanket per litre water.
- The recirculation ratio is a coefficient for the amount of water that is recirculated.
 This water is recirculated to achieve a higher inlet concentration which improves sedimentation.
- The initial settling velocity is the velocity in the y-direction of the particles entering the tank.

3.3 CFD Packages available and used

To learn to use CFD software packages requires a great deal of time and effort. Not only must the commands and facilities of each particular package be mastered, but also the skills required to develop suitable grids and speed up convergence or stabilization of solutions.

There is a great variety of software packages available. Not all of them are equally suitable for simulation of sedimentation tanks. Initially CFD software was developed to simulate gas (usually air) flow over objects, e.g. to streamline designs for motor cars or aeroplane wings. From there it evolved into simulating flow of liquids, chemical reactions and flow with interactions between different phases of matter. To simulate sedimentation tanks, for example, requires physics and mathematics to describe the interaction of a solid phase (flocs) with a liquid phase (water). Added to this is the fact that water is an unusual liquid, with a high viscosity relative to its density due to hydrogen bonding between its molecules. Not all CFD packages include the necessary algorithms to deal with these aspects.

It would also be prohibitively expensive and time-consuming to evaluate every available package on the market. To learn to use these software packages requires a great deal of time and effort. Because of this it was necessary to make an early selection of a suitable package.

Flo++

The Flo++ computational fluid dynamics software from SoftFlo was used in this investigation. Le Grange developed Flo++ during the 1990's in Potchefstroom, South Africa. Flo++ is based on the finite volume method and uses the SIMPLE algorithm to solve the three-dimensional transport equations. It was selected because the full functional software package and support was available to the researchers at minimal cost, since it is developed locally. It is also readily available to other researchers at a reasonable cost. A fairly powerful demonstration verrsion can be downloaded free of charge from the company SOFTFLO's web site at http://www.softflo.com. The demonstration package is limited in the number of computational cells and does not allow user coding. When this project was started, version 2.3094 was available. In 2002 a major new version was released and version 3.07 was used for the simulations of the Midvaal plant's tanks. The biggest change was in the pre- and postprocessor interface.

Other packages

One of the researchers on this project (Du Toit) also has experience of working with StarCD, a package from the UK. Some of the other researchers also received training on it. It is very similar to Flo++, the latter having been modelled on it to a large extent, although it does not use the same code. However, it is much more expensive than Flo++. Some work was done with it during this project, but with Flo++ backup service was more readily available to us.

Fluent is mentioned a number of times in the literature. Amongst others, it was used by Brouckaert *et al* (2000) to model an ozone contactor at Wiggins Water Works in a WRC project that ran concurrently with this one.

Krebs (1991) used the **PHOENICS** code to show the qualitative effect of various geometrical changes. He showed that inlet baffles, dividing walls and energy dissipating devices can increase tank efficiency. Dahl et al.(1994) used the PHOENICS code to simulate a laboratory sized secondary settling tank. Comparisons with experimental horizontal velocities and solids concentration showed good agreement.

Frey et al. (1993) used the VEST code to determine the flow pattern in a sedimentation tank as input for the TRAPS code which determined particle tracks.

A number of CFD demonstration packages are available as downloads from the Internet.

4. VALIDATION OF CFD MODELS OF RECTANGULAR SEDIMENTATION TANKS

4.1 Benchmarks and validation criteria

In order to determine whether CFD is a reliable method to do modelling and simulations of sedimentation tanks, it is necessary to have a standard against which it can be validated by comparing the simulated cases with physical experiments. This was done it by using a physical small scale laboratory model of such a tank, called the labtank. Experiments were conducted with this model, and these experiments were then simulated with CFD using Flo++ in order to determine whether the simulations showed good correspondence with the physical experiments.

It was also necessary to ensure that the physical experiments mimic the operation of full scale sedimentation tanks realistically. In order to ensure this, it was necessary to set some performance indicators for the labtank (physical) experiments, the CFD simulations of the labtank and the CFD simulations of full scale tanks. As a first step to do the last, use was made of the Jönköping tank at Lund, Sweden. As stated previously in paragraph 3.3, this is a well-studied case that is used as a benchmark for similar work. Van der Walt (1994) did this for his M.Eng. thesis and obtained good results. Because he used an older, DOS-based version of Flo++ and to gain experience with CFD and Flo++, some of his work was repeated.

Van der Walt also used Flo++ as an aid in designing the new settling tanks at the extension of the Vaalkop plant of Magalies water in the year 2000. The experience at the plant since also validated the design work.

On the basis of these positive results, it was decided to also do simulations of the tanks at the Midvaal purification plant, Orkney with Flo++. These results were not validated by any measurements or data in the time frame frame of the project, but did not yield anything physically unreasonable and corresponded well with the experience and observations of the staff at the plant (e.g. in respect of the effect of wind and water temperature).

The abovementioned were the most important steps in the process, but it was also necessary to set criteria for subsystems or components in the modelling and simulation process. An example is the criteria set for the particles and materials used to simulate flocs in the labtank. This was done after an initial trial and error process made it clear that such criteria was necessary.

Indicators for the labtank experiments.

- Are the experiments repeatable?
- 2. Do the water flow patterns through the labtank resemble those in full scale tanks?
- Do particle trajectories resemble those in full scale tanks? (As can be observed in the inlet cloud, in the proportion and sizes of particles carried out of the tank at the outlets.
- 4. Are Froude numbers of the correct magnitude?
- 5. Does the flow patterns in the tank stabilize (whether steady or unsteady) during experimental runs?
- 6. Do changes to operating parameters during runs lead to expected and realistic behaviour in the labtank?

Indicators for CFD simulations of the labtank.

- 1. Do the flow patterns in the simulations correspond to that in the physical experiments?
- 2. Do the particle trajectories correspond to the physical experiments?
- 3. Do flow velocities at different parts of the tank correspond?
- 4. Do the simulations yield similar solids concentrations in various parts, especially the outlets?
- 5. Are the modelling assumptions and simplifications valid (or is 'backward engineering' required to get realistic results)?

Indicators for CFD simulations of full scale tanks.

- 1. Are the simulations realistic, i.e. do they correspond with what is known of/about the behaviour of the full scale tank in terms of flow patterns, particle settling patterns, floc clouds at inlets, particle concentration in effluent?
- 2. Are the modelling assumptions and simplifications valid?

3. Do the simulation results correspond to that of the labtank simulations, i.e. do similar changes in operating parameters cause similar effects?

4.2 Variables investigated.

In this paragraph the input and output variables to both numerical and experimental models are defined and described. The experimental and numerical models are described, along with the desired results from them. The influence of tank geometry on solids removal rate were investigated physically and numerically. Numerical results were correlated with physical measurements.

Results required from the Labtank:

- Observation, photographs and drawings indicating the water flow patterns and particle trajectories inside the tank.
- Observation of the effect of changing the tank configuration at the inlets (including baffles) and outlets.
- Investigation of the effect of changing operational parameters (water flow rate; water temperature; particle concentration; particle size distribution; particle density).
- · Validation of the CFD simulations of the labtank using Flo++.

Input variables to laboratory experiment:

- Volume flow rate into tank
- Sludge concentration C_{in}
- Average particle diameter d_p
- Water temperature T_{in}

From the water temperature the density and viscosity of the water cuold be calculated.

The numerical models for settling tanks required the following physical data:

Fluid momentum model:

Water density and viscosity ρ_w μ

(Determinable from temperature - Appendix C: Properties of water)

Inlet velocity into settling tank u_{ij}

Particle tracking model:

- Inlet solids concentration C_{in}
- True density of flocs in water ρ_p
- Mean particle diameter d

4.3 The laboratory model tank (Labtank)

Physical configuration.

A scale model of a rectangular settling tank was used to validate and calibrate the numerical model. This will be referred to as the labtank. The labtank was built completely from clear perspex so that flow profiles could be observed and photographed in detail. It was designed so that inlet and outlet geometries can be changed very easily. The flow domain in the labtank is outlined in Figure 4.1. See Appendix A for a geometric description of flow domain in the labtank.

The water delivery system to the labtank featured:

- · Temperature measurement
- · Continuous volume flow rate indication
- · A tracer (dye) injection point

(See Appendix B for a description of the water and sludge delivery system.)

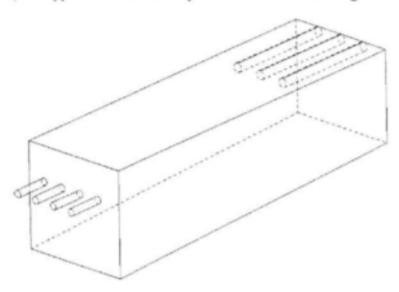


Figure 4.1 Outline of the flow domain in the Labtank.

4.4 Simulation of floc particles in the Labtank.

4.4.1 Requirements

The material used to simulate the floc particles in the labtank had to fulfil the following requirements:

- It must be inert, i.e. not be affected chemically by the processes occurring in the simulation process, e.g. the addition of tracer. This also makes it possible for it to be recovered and reused for subsequent experiments. It must also not be toxic, because some of it inevitably escapes during the course of the experiments, it has to be handled manually and it also has to be disposed of eventually.
- It must be stable, i.e. not be affected physically by the processes occurring in the simulation process. For example, it must not break up into smaller pieces or absorb water into its physical structure, thus changing its size or density during the course of an experimental run.
- It must be characterizable, i.e. it must be possible to specify its size, shape and density, and either measure or calculate its settling velocity to reasonable accuracy for experimental purposes and as input to the numerical model.
- It must be visible in the tank for visual observation and photographic recording, with and without tracer added.
- It must be realistic, i.e. its size, shape and density should be similar to that of typical floc particles in order to ensure that the laboratory simulations are realistic.
- Its motion through the water in the tank should correspond to that of flocs.
- 7. It should be inexpensive.

It was difficult to fulfil all these requirements and various substances were tried as simulants for flocs during the course of the research project.

4.4.2 Materials tried as floc simulants.

A study of literature on the subject showed that researchers used a great variety of substances and materials to produce or simulate flocs for experimental purposes. Haarhoff et al (1996) made use of synthetic kaolin suspension. They do not specify the flocculant used. Elmaleh and Jabbouri (1991) used a synthetic bentonite suspension dosed with ferric chloride solution. Cornelissen et al (1997) used solutions of ferric (III) sulphate hydrate with nitric acid and added sodium hydroxide, which proved to be unstable over time, so it was replaced with Fe stock solution, stabilized with 1% conc. sulphuric acid, which was stable over time. Vlaski et al (1997) used the cyanobacteria Microcystis aeruginosa. Tambo and Hozumi (1979) used kaolinite clay dosed with alum. Logan and Kilps (1995) used fluorescent carboxylate microspheres (type YG, Polysciences Inc.). Chen (1998) used kaolin clay flocculated with nonionic, cationic and anionic polymers.

At first it was attempted to use kaolin obtained from a pharmacy in suspensions dosed with Fe(OH)₃, Al(OH)₃ or polyelectrolytes to prepare floc particles for the experimental tests in the labtank. This attempt was unsuccessful, because it was found to be impossible to repeatably prepare batches of flocs with the same physical characteristics and settling rate (especially of the same size) in sequential preparation batches.

Next it was attempted to prepare flocs using solutions of Fe(OH)₃, Al(OH)₃ and lime. Again it was not possible to obtain repeatable results.

Sago grains were tried next, but it absorbed too much water and became sticky. These changes in its physical characteristics made it unsuitable.

The idea was then conceived to used maize meal. This fulfilled most of the requirements. Although it is not completely stable and inert, its characteristics did not change significantly during the course of an experimental run, and it is so inexpensive and available that it could be discarded after an experimental run. It could also be coloured blue to increase its visibility by dosing it with iodine solution before adding it to the water, although the colour faded rapidly during the experiments in which this was tried. Unfortunately some of it always remained somwhere in the equipment where it quickly became putrid. At 1410 kg/m³ its density was on the high side to be really realistic and also affected the Froude number.

Finally it was decided to use crystalline polystyrene, ground to the required size. This fulfilled all the requirements and was used succesfully in the experiments thereafter. The s.g. of polystyrene is given in the Handbook of Chemistry and Physics (Weast, 1979 p C-785) as 1,04 – 1,08 and we determined the density of our own sample as 1013,031 kg/m³, which is usable for this type of simulation, although a bit on the low side. Grinding it to smaller sizes was a problem. If the right type of equipment was not used, it tended to melt and stick. A steel ball mill worked best. It was highly surface active after grinding and refused to settle initially, but after treatment with the surfactant sodium lauryl phosphate, it settled very realistically.

Both the maize meal and polystyrene particles were sieved to determine size distribution and to segregate it into particles of suitable size ranges for the different experimental runs.

5. TYPICAL RESULTS AND PRESENTATION OF CFD SIMULATIONS

5.1 The standard case of the tanks.

The purpose of this chapter is to illustrate the typical results of CFD simulations. The examples used in this section (5.1) are from the simulations done on the standard case of the sedimentation tanks at the Midvaal purification plant. The results of simulations to investigate the effect of changes in configuration and operational parameters at Midvaal are presented in chapter 7.

CFD simulations can be used to see literally an infinite number of views of a subject of study. Apart from the fact that the operational conditions of physical configuration can be adjusted before doing a simulation, the following can be done by means of the post-processor once a solution is obtained:

- A cross section can be viewed in any of the three spatial dimensions through any
 of the cells in the mesh.
- 2. It is possible to zoom in on part of the subject to see it in greater detail.
- The colour scale can be adjusted to provide information at a different range of resolution.
- Different types of views can be selected, e.g. velocities can be viewed in contour
 plots to show areas of different intensities, or as vectors. These different types can
 be combined with different views of the mesh.
- Particle trajectories can be viewed at different time intervals to show their development, as well as phenomena like trapping of the particles in certain flow regions.

All of the above were used during this project and will be illustrated in what follows.

It demonstrates the power and convenience of CFD. (The caveat is that it must be ensured that the simulation is realistic.)

Note: CFD yields vast amounts of information that has to be viewed as graphics in colour or grayscale tones to comprehend. Because of this, most of the graphics in this and the following chapters are not included in the text. To include it would have made the report too bulky and difficult to cross refer. Instead the figures are provided on the CD ROM as files that are referred to in the text and can be opened on the computer for viewing. The naming

convention for these files are fx_y, where the single f indicates that the file is on the CD, x is the relevant chapter number and y the figure number.

Figure f5_1(a) [i.e. file f5_1 on the CD ROM] shows a typical view of a contour plot of the velocities at a cross-section through the z-axis. (NB it is a cross-section, not a side view!) Because of the values on the colour scale, 90% of the tank's volume falls into the lowest range of the scale, showing no detail of the flow at the outlet area, or possible short-circuiting through the settling zone of the tank. Also, the view is too small to discern much at the inlet zone. Figure f5_1(b) is the same view, but zoomed in to show detail of the flow at the inlets. (The view is a cross-section between the two centre inlets.) Figure f5_6 is a similar view, but at a different cross-section. Figure f5_1(c) is a view from the top (y-axis) side, with the section one third from the top of the tank.

The different cross sections used are shown in figure 5.1 on the next page. Section A is the standard one, corresponding to figure f5_1(b); section B corresponds to figure f5_6 and section C to figure f5_1(c).

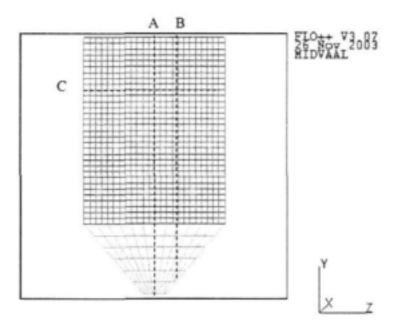


Figure 5.1. Cross-sections (planes) used in the figures.

Figure f5_2 (b) shows the velocity vectors, i.e. the direction of the flow, in the centre of each cell. The magnitude of the velocity is represented by both the colour scale

and the arrow length. Note that the range of the scale for the vector plot differs from that of the contour plot. On the vector plot it can clearly be seen that the placement of the inlets causes a very strong vortex to be formed in the inlet zone.

The effect of this vortex on the particle trajectories is shown in figure F5_2(c). The view displays the trajectories of particles over a period of 10 minutes. The colour scale is ranged between the diameter of the smallest and largest particles, which in this case were the only two sizes specified, viz.1 and 2 mm respectively. The whole range of colours on the scale is not necessary for this case, but will be useful if a larger size distribution is specified in the pre-processor, especially if the distribution is not in directly proportional sizes. Only the trajectories of particles that have not settled out are displayed. Quite clearly a significant portion of especially the 1mm diameter particles are trapped for very long times in the inlet vortices. To show this more clearly figure f5_5 shows the development of the particle trajectories after time periods of 60, 300 and 600 seconds (1, 5 and 10 minutes) respectively in (a), (b) and (c). The presence of a weaker secondary vortex inside the first sludge sump is also observed in (b) and (c). It can also be seen in the vector plot of figure f5_2(b), but not as clearly.

This trapping and continuous recirculation of the particles in the vortices in the inlet zone explains why a clearly delineated floc cloud, almost like a sludge blanket, can normally be observed in the inlet zones of rectangular sedimentation tanks. If the particles are indeed trapped in this zone for such extended time periods, it can have significant beneficial or detrimental effects on the efficiency of the tanks. On the one hand the particles can be subjected to high shear stresses, causing the floc particles to break up, thus reducing efficiency. This is unlikely because the highest velocities and shears are experienced right at the inlet openings. On the other hand, the recirculation effectively increases flocculation time and the shape of the vortices causes tapered G-values in their vicinities, creating good conditions for further flocculation. It is thus likely that at least some of the flocs will agglomerate further until they either move into a region of lower velocity or become heavy enough to drop out of the vortices. This will increase efficiency. It will be worthwile to investigate this further.

To see how far the inlet zone really extends, and also what happens at the outlet zone, the colour scale range was changed so that the maximum value is 10 times smaller, i.e. 3.1×10^{-2} m.s⁻¹. If the inlet zone is defined as the volume in which the flow is influenced significantly by the inlet jets and the settling zone as that in which the flow has become evenly distributed in depth and length, then figure $f5_3(a)$ shows that the inlet zone forms 24% of the tank's volume. The actual settling zone forms 66% of the tank. The outlet zone consists of the remaining 10%. For this tank only the volume directly at and below the outlets are affected by the presence of the outlets (figure $f5_3(b)$)

Figure f5 3(c) is interesting because it shows a shortcoming of CFD. In order to reduce computing time and hardware requirements, use is made of symmetry. As explained in chapter 4, a mesh of only the middle section was constructed for the Midvaal simulations. It was then specified that the mesh is symmetrical on both sides of it. This is not really true, for two reasons: Firstly, the tank has got side walls. However, it was assumed that the effect of the sides on the flow will be limited to the vicinity of the walls due to the low flow velocities. This is a reasonable assumption. Secondly, the inlet pipe and outlet channel configuration is not really mirrored at the symmetry boundary as can be seen in figure f5_3(c) - the inlets form a zig-zag pattern. Assuming symmetry here means that at the symmetry boundaries there will be discrepancies in the distances between the inlet pipes and between the outlet channels. The effect of this can also be seen in figure f5 3(c), where the section view from the top (y-axis) was selected to show the worst inaccuracy in the solution caused by it. It can be seen that there appears to be a spot of significantly higher flow at the one end of the upper outlet channel. This is not the case in reality - it is caused by the (not shown) presence of the next outlet channel, which is closer to it in the simulation than in reality, causing the increased outflow in this region.

Except for the artefact caused by this inaccuracy, the realism of the simulations were not affected. This raised the question whether the design of the outflow channels or outlets had such small effect on the flow patterns and efficiencies of rectangular tanks in general. This was investigated with simulations of different outlet configurations for both the labtank and Midvaal tanks. The results are presented in the next two

chapters. It was observed in both cases that the effect of radical changes in outlet configurations did have much less effect on flow patterns than changes in inlet design.

5.2 Comparison of simulation of 2-phase flow using scalar and discrete algorithms

A simplified model of the Jönköping tank (Larsen, 1977) was modelled to investigate settling of particles. It was also used for validation by comparison with the published results, especially those of Van der Walt (1994). Van der Walt used version 1.5 of Flo++, which is DOS-based, whereas both versions of Flo++ used during this project were developed for versions of Microsoft Windows.

Van der Walt used a scalar approach to simulate the solid phase because simulating discrete particles was not feasible at the time due to hardware constraints. (He used a 486 computer with 32 Mb RAM.) When this study used a scalar simulation, the results for the distribution and concentration of the particles didn't agree with those of Van der Walt. Figures f5_6A and f5_6B show the concentration of the particles of Van der Walt's model and of the current model.

This discrepancy is due to the fact that Van der Walt used a specially coded boundary condition for the bottom wall to make provision for the sludge. This code was compiled into the Flo++ code for him by the developer and was not available for this study, therefore it was decided to concentrate on two-phase modelling using discrete particles, since this option had become viable due to the development in personal computer hardware in the meantime.

The flow in the tank compared reasonably well as can be seen in Figures f5_7A and f5_7B. The velocity ranges as well as the contours compare reasonably well.

Particle tracking

Models were developed and run with scalars as well as with particle tracking. The results for the flow correlated very well, as can be seen in Figures f5_8A and f5_8B.

Summary of results

- The water jets at sedimentation tank inlets cause vortices to form, which trap and recirculate particles in the inlet zones, forming the characteristic floc clouds in them. These floc clouds probably affect the particle settling and therefore tank efficiency.
- The presence of the solid phase (floc particles) in inlet zones causes density waterfalls to develop because the particles interact with the water due to their weight and drag forces.
- The inlet zone in general can be characterized as that volume of the tank in which
 the water flow patterns are determined completely by the inlet jets and particle
 density waterfalls.
- The simulations done in this project showed good agreement with benchmarks like the Jönköping tank. Different approaches for modelling the same aspects also correlated well, except for sludge concentration profiles using discrete particles.

6. CFD SIMULATIONS OF LABTANK

6.1 Development of the numerical model

6.1.1 Computational mesh development

At first, a three-dimensional model of the tank, consisting of 39 864 cells, was used to model the labtank. See figure 6.1.

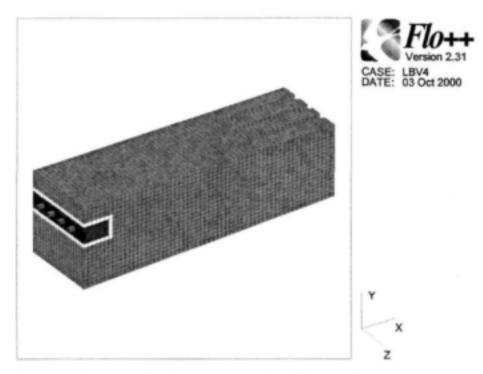


Figure 6.1 Three dimensional computational grid of the Labtank.

However, the computational effort to solve such a large model made it inappropriate for this study. A pseudo two-dimensional model of 1300 cells was then employed. A section of 2mm thick was taken through one of the inlets. It is a pseudo 2-dimensional model because the finite volume method is used and the cells must have three-dimensional volume. However, the mesh has a thickness of only one cell. This is then considered as a two-dimensional model, because the flow is calculated on a grid with only two dimensions. This is shown in figure 6.2.

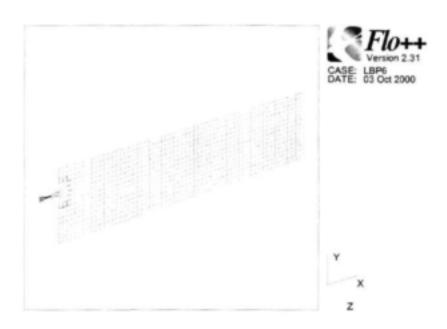


Figure 6.2 Two dimensional computational grid of the Labtank

The mesh at the inlet had to be refined to give a smooth transition from a fine grid to a coarse grid. Detail at the inlet of the grid in figure 6.2 is shown in figure 6.3. The inlet configuration as shown was used when maize flour was utilized as a floc simulant. Due to its higher density than that of the crystalline polystyrene used later during the experiments the inlets had to have a reduction in diameter to maintain the same .Freude number. This was changed back to the design shown in figure 6.8 later.

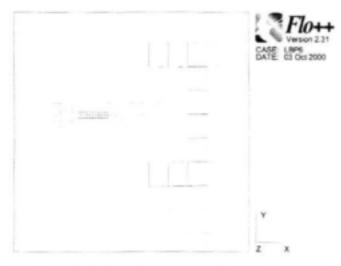


Figure 6.3 Grid refinement at the inlet of the two-dimensional mesh.

6.1.2 Relaxation parameters

The relaxation parameters required for the neutral density flow were also investigated. Results confirmed the information on relaxation parameters presented by Ferziger and Peric (1996). Graphs from their research are shown in figure 6.4. The relaxation parameter combination yielding the quickest stable reduction of the residuals were 0.8 for velocity and 0.4 for pressure for our models.

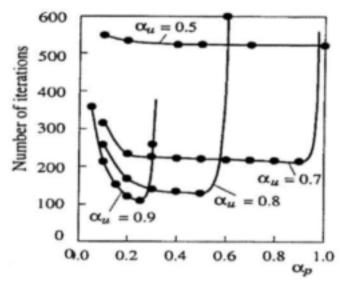


Figure 6.4. Number of iterations required to reduce the residual level in all equations three orders of magnitude using various combinations of under-relaxation parameters and a 32x32 uniform numerical experimental grid with co-located arrangement of variables.

 α_a : velocity relaxation α_p : pressure relaxation.

(From Ferziger and Peric 1996)

6.1.3 Simulation of floc behaviour

When the inlets were modelled, it seemed a natural choice to place the particles in the inlet. That would ensure a realistic simulation. However, as happened with the real labtank, particles settled in the inlet and the model did not converge. Convergence of a coupled particle tracking model was found to be much more dependant on mesh attributes than a neutral density problem. Figure 6.6 shows a mesh that was used initially. Figure 6.7 shows the particle tracks the mesh in Figure 6.6 gave after 5000 iterations. Just the particle tracking time was changed in each case, showing that the solution was completely unstable.

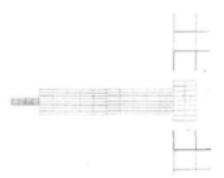


Figure 6.6 Initial mesh of inlet

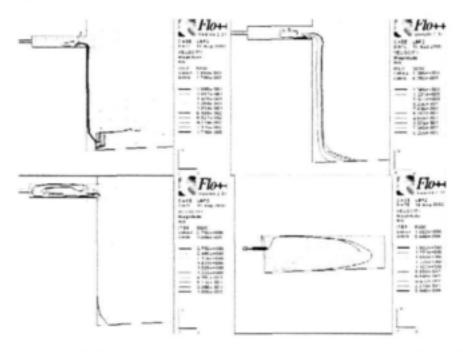


Figure 6.7 Erratic particle tracks resulting from the mesh in figure 6.6. In the different cases, only the frequency of particle tracking was changed.

This problem was due to the aspect ratio of the inlet cells (Le Grange, 2001). The aspect ratio is the ratio between the length and width of the cells. After changing the aspect ratio of the cells to 1, the model converged in 468 iterations. The changed mesh is shown in figure 6.8. The results obtained using this mesh are shown in figure 6.9.



Figure 6.8 New computational mesh with aspect ratio of cells at a value of 1.

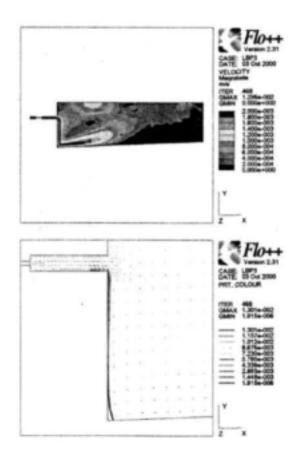


Figure 6.9 Velocity contours and the particle tracks resulting from the mesh in figure 6.8.

The final CFD grid of the labtank that was used in the simulations was a section comprising a third of the tank, cut lengthwise, with symmetry boundaries specified on the sides, as shown in figures 6.10 (a) and (b).



Figure 6.10(a) Final CFD mesh of labtank model.

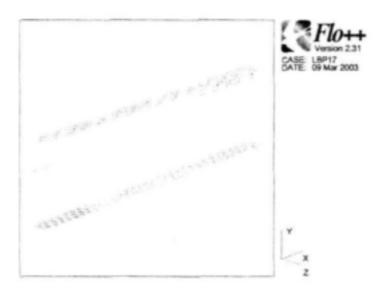


Figure 6.10(b). Boundary configuration.

6.2 The standard case simulation of the Labtank.

6.2.1 Parameters for standard case

Particles:

Concentration: 12,5 g/l

Density $\rho = 1014 \text{ kg/m}^3$ (crystalline polystyrene)

Diameter: φ = 400, 500 & 600 μm

Fluid:

Temperature T = 21 °C

Density $\rho = 9.98 \times 10^2 \text{ kg/m}^3$

Viscosity: 0,9994 x 10⁻³ Pa.s

Inflow rate: 1,85 l/min

Inlet configuration:

Inlets: 4 inlet pipes of diameter 20 mm equally spaced in a horizontal row.

Outlets consists of three channels, each with five holes equally spaced on each side.

No baffles.

6.2.2 List of figures with parameters changed during the respective simulations:

f6_1: Labtank standard case

Particles:

f6_2: Effect of particle concentration

f6 4: Effect of particle diameter

Fluid:

f6_5: Effect of fluid temperature

f6 6: Effect of inflow rate

Inlet configuration:

f6_7: Effect of baffles

Figure f6_1 shows the results of the simulation for the standard case, as well as for that without particles in the water. The view in this case is through a plane right through one of the baffles in the middle of the tank. (The smaller blocks at the inlets are not walls or boundaries, but the limits of volumes in which the computational mesh was refined to obtain better numerical stability and detail resolution, as can also be seen on the vector plot.) It shows that the jet of water at the inlet causes two vortices to form, one below the jet and one above it. The area that is influenced by

the inlet jet and its associated vortices (the inlet zone) consists of ca 27% of the total tank volume.

Quite enlightening was the fact that the splitting of the particle trajectories in "curtains", as observed in the simulation did indeed take place in the physical experiments, although only at temperatures higher than 15°C. This was a good example of the CFD model behaving realistically, although not deterministically, and served to increase confidence in its use.

6.3 The effect of changes in the operational parameters.

Particle concentration:

As with the Jönköping tank, but unlike the Midvaal tanks, the particles have a very significant effect on the water flow pattern inside the tank. With particles present, a very strong density waterfall develops in the inlet zone, changing the relative sizes and shapes of the inlet vortices to the extent that the left-turning vortex becomes dominant when particles are present. This effect is dependent on the concentration of the particles, as can be seen when comparing figure f6_1 with figure f6_2, which shows the effect of increasing particle concentration. (The particle concentrations had to be so high in order to obtain realistic models by maintaining realistic Froude numbers at the inflow.) At 8 g/l the two vortices are about equal in extent and velocity; with increased concentration, the left turning one becomes increasingly dominant.

Particle diameter:

In the simulations shown in figure f6_4 different particles were used, keeping the concentration constant at 12.5 g/l. As expected particles with different diameters followed diverging trajectories; the more different the diameters, the more divergent the trajectories. Because of this spatial 'spreading' out of the particles, the shape of the density waterfall was also affected.

Water temperature:

As discussed earlier, changes in water temperature affect the density and viscosity of the water. This in turn has an impact on the settling rate of the particles. To investigate this simulations were done at four different temperatures, viz. 4, 11, 21 and 25°C. Results are presented in figure f6_5. At the higher temperatures the numerical solution took longer and for 25 °C a steady state solution could not be obtained. At first this was thought to be a numerical problem, but physical experiments on the labtank confirmed that at higher temperatures the flow was unstable and switched between different states. Again the CFD model behaved realistically.

Inflow rate:

Changing the inflow rate from 1,85 to 2,2 l/min, i.e. an increase of 19%, did not affect the flow pattern and particle trajectories significantly, although the flow velocities did increase. This stability of the flow pattern to changes in flow rate was also observed in the Midvaal simulations.

6.4 The effect of changes in the tank configuration.

Adding a baffle:

Baffles were added to the labtank at different distances from and also at different angles to the inlets. An example of the results is given in figure f6_7. In this case it had the effect of flattening the vortex towards the inlet in order to contain it in front of the baffle. It also increased the recirculation of particles by the right-turning vortex in the lower left corner, compressing the particle settling footprint slightly in the process. The same effect was again observed in the physical experiments, but much more so than in the numerical solution. The numerical solution developed much more slowly than in the standard case.

Changing inlet configuration:

Instead of 4 inlet holes in a row, the inlet pipes were spaced rectangularly. The result is shown in figure f6_8. It caused the two layers of inlet jets to interact and converging to one another due to the low-pressure region between them. This caused the density waterfall to become narrower instead of broader as it flowed to the bottom and also decreased flow velocities in the inlet zone. It also caused the inlet jet to become elongated along the bottom of the tank. This effectively increases the volume of the inlet zone relative to the rest of the tank and will probably have a negative impact on tank efficiency in practice, although it did not increase particle outflow at

the outlets in the labtank experiment. This was probably due to the relatively large particle sizes, causing the particles to settle out. The settling footprint did extend further into the tank after the labtank experiment, confirming the realism of the simulation.

Summary of results

- Developing a suitable mesh for CFD simulations is the most time-consuming part
 of the work. A suitable mesh is one that provides simulations that are independent
 of the mesh itself, are stable and repeatable and yields results within useful
 timeframes.
- Pseudo two-dimensional grids are not suitable for simulations involving discrete particles.
- Grid refinement at the inlets and outlets are necessary to obtain adequate resolution and to allow the flow to develop sufficiently for solution stability to be achieved.
- The relaxation parameter combination that yielded the quickest stable reduction of the residuals were 0,8 for velocity and 0,4 for pressure, which corresponded to values found in literature.
- For discrete particle modelling, it was necessary to keep the aspect ratio of the mesh cells at one, otherwise the calculated particle trajectories were erratic.
- The labtank simulations were very realistic and gave qualitatively similar results to the physical experiments, For example: in both the simulations and experiments the particle trajectories in the density waterfall developed a nonsteady pattern appearing like curtains moving in a breeze. The temperature also affected the simulations and models in similar ways.
- Baffles did affect flow patternsin the tank similarly in simulations and experiments. In both cases the effects were confined to the inlet zone, with no significant influence on either the settling or the outlet zones.

7. CFD SIMULATIONS OF MIDVAAL TANKS

7.1 Development of the computational mesh.

Geometry of CFD mesh of Midvaal tank.

The following mesh was developed to simulate the full-scale Midvaal tank at Orkney in the North West province. As in the case of the labtank (chapter 6), the mesh represents the middle third section of the tank, with symmetry on the sides.

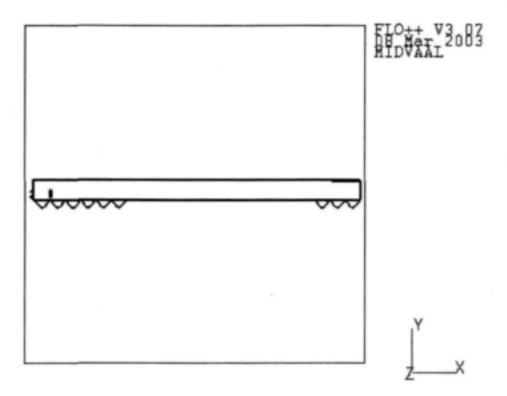


Figure 7.1 Side view of Midvaal tank (also showing baffle).

In order to have a model that was independent of the mesh and to improve the resolution, it was necessary to refine the mesh at the inlets and outlets. Therefore the mesh was constructed as a combination of nine different blocks (sections) consisting of different sizes of cells in order to obtain the best resolution and numerical stability with the least computing requirements.

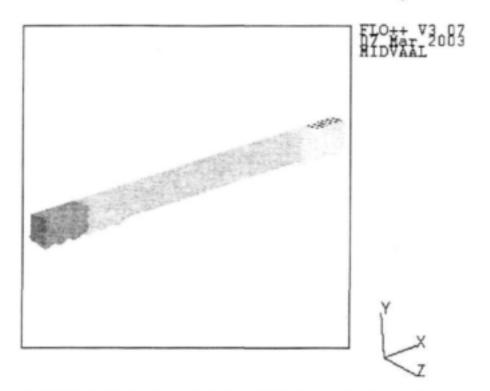


Figure 7.2 Computational mesh for the standard case of the Midvaal tank.

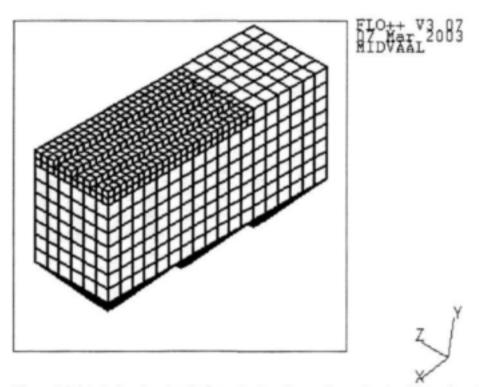


Figure 7.3 Mesh showing detail of standard outlet configuration for Midvaal tanks.

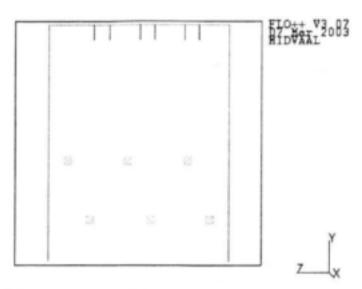


Figure 7.4 Detail of inlet and outlet configuration for Midvaal tanks.

7.2 The standard case of the Midvaal tanks.

A CFD model was first developed to simulate the existing configuration and most usual operating conditions of the Midvaal tanks. This model was then adapted to investigate the effect of changes in configuration or operating conditions in subsequent simulations. The parameters for the standard model were the following:

Particles:

Concentration: 10 mg/l

Density $\rho = 1200 \text{ kg/m}^3$

Diameter: $\phi = 1000 \& 2000 \mu m$

Fluid:

Temperature T = 11 °C

Density $\rho = 9.996 \times 10^2 \text{ kg/m}^3$

Viscosity: 1,270 x 10⁻³ Pa.s

Inflow velocity $u_x = 1.67 \text{ m/s}$

No wind

Inlet configuration:

Without baffles

Inlets at bottom

As in the previous two chapters, the results of the different simulations are stored on the CD ROM as files to be accessed as referred to in the text. They are:

f 7_1: Midvaal Standard case

Particle features/charateristics

f7 2: Without particles

f7_3: Particle concentration = 25 mg/l

f7_4: Particle concentration = 10 g/l

f7_5: Particle density = 1500 kg/m3

f7 6: Particle diameter = 300 & 600 μm

Fluid characteristics

f7_7: Fluid temperature = 21 °C

f7 8: Inflow velocity 70 % of standard

f7_9: Inflow velocity with y-component of 5 % of x-component

f7_10: Wind x = +1 m/s (from inlet to outlet)

f7_11: Wind x = -1 m/s (from outlet to inlet)

Inlet configuration

f7_12: Without first three sumps

f7_13: With baffle

f7_14: Inlets in middle

f7_15: Inlets at top

f7_16: Inlets at top (different colour scale)

f7_17: Outlet configuration

f7_18: Inlet and outlet configuration (changed simultaneously)

Note: All the views in the graphics included in this chapter are of cross-sections through the plane A as shown in figure 5.1, chapter 5. All the particle trajectories are shown for time periods of 600 s (10 minutes). Only trajectories of particles that have not settled out are shown. It is also important to note that the velocity contours and

vectors are views through planes, but that the particle tractories shows **all** particles in the whole 3-dimensional space.

7.3 Effect of changes in operational conditions.

Without particles:

Figure f7_1 is a representation of the standard case, as discussed already in chapter 5. The first variation was to do the simulation without floc particles present in the water. The result is shown in figure f7_2. Unlike the simulations of the Jönköping tank and the labtank, the particles do not have an observable effect on the flow patterns in the tank. This initially surprising result can be ascribed to three reasons:

- The flow rate at the inlets of the Midvaal tank is an order of magnitude higher than in the labtank. This makes the inlet jets and vortices much stronger.
- The particle concentration in the Midvaal tank is 3 orders of magnitude lower than in the labtank. (The concentration in the labtank had to be so high in order to obtain the correct Froude number at the inlets.)
- Contrary to the Jönköping tank and the labtank, the inlets at the Midvaal tanks are situated at the **bottom** of the tanks and not in the upper half. Together with the much higher flow rate this prevents a density waterfall from developing in the inlet zone.

Changing particle concentrations:

Figure f7_3 shows the effect of changing the particle concentration to 25 mg/l, and figure f7_4 an increase of 3 orders of magnitude to 10 g/l. The last was done to see if this could force the development of a density waterfall. As can be seen in both figures in comparison with the standard case (figure f7_1) these changes did not affect either the flow patterns or velocities significantly. At the highest concentration there was some change in the particle trajectories in the inlet zone and the flow through the second and third sumps due to the development of a relatively weak density waterfall in this region as can be seen on the trajectory and contour plots.

Increasing particle density from 1200 to 1500 kg/m³ (Figure f7_5):

This did not have a significant effect on flow patterns and velocities, or on particle trajectories.

Decreasing particle diameters from 1000 and 2000 μm to 300 and 600 μm (Figure $f7_6$):

Again this did not have a significant on flow patterns or velocities. It did have a very significant effect on the particle trajectories. Since only the trajectories of particles that were not removed after 10 minutes are shown, it can be observed very clearly that especially the smaller particles have been removed from the tank, either by settling out or by being carried out. They did not become trapped in the vortex to the same extent as the larger particles, because they are swept into the settling zone of much lower velocities.

The flow patterns and velocities in the Midvaal tanks showed remarkable stability in terms of the effect of changes in particle characteristics, especially when compared to the labtank. The fact that it can accommodate such a variation in particle density, diameter and concentration suggests that other particle characteristics like floc particle composition and shape are less significant in terms of flow than expected in comparison to hydraulic parameters.

Changing operating temperature from 11 to 21 °C (Figure f7 7):

This temperature change changes the density of the water from 999,6051 to 998,0347 kg/m³ and the dynamic viscosity from 1,270 to 0,9994 x 10⁻³ Pa. (see Appendix C). The density decreases by 0,16% and the viscosity by 21,3%. This will obviously effect the settling rate of the particles (see section 2...2.2), but what will be the effect on flow patterns? Figure f7_7 shows that the flow patterns were not affected by the temperature change. The particle trajectories were influenced, but not to the extent expected.

The temperature did affect the computation of the solution. The number of iterations to convergence increased by 44%. This is due to the reduction in water viscosity, making the flow less "stiff" and therefore more unstable, which is reflected in the computational stability.

Reducing the flow rate by 30% (Figure f7_8):

This decreases the flow velocity at the inflows by 30%, affecting the inflow jet and vortices. As can be seen in figure f7_8, the flow patterns were not changed by this, although the flow velocities were. (If the colour scale range is adjusted proportionally the velocity contours and vectors appear the same.) Particle trajectories were also influenced, with more particles settling out in the 10 minute interval, as can be expected.

Adding a downward component to the inlet velocity (Figure f7 9):

In reality the inlets consist of pipes going down the walls at the inlet side, with 90° elbows at the end to inject the water parallel to the surface and not downwards. It is possible that this causes the momentum to have a component in the –y direction. A simulation was done with a y-velocity component of 5% of the x-velocity at the inlets. Figure f7_9 displays the results. The influence on the flow pattern was slight, that on the particle trajectories more significant. Fewer particles were trapped in the inlet vortices and the particles followed a more uniform trajectory towards the settling zone.

Again it was observed that the flow patterns in the tank are remarkably stable to changes in the fluid flow parameters, as in the case of changes to the particle characteristics. From this perspective it is a very good design. Operational experience at the plant confirms this. (Pietersen, 2003.) The tank can be relied on to yield water with a turbidity of between 2 and 3 NTU. The plant also has circular tanks. The water produced by them can have somewhat more variation in turbidity (between 0,5 and 5 NTU), although normally it is lower than that from the rectangular tanks.

Effect of wind:

It is well-known that wind affects the operation and efficiency of sedimentation tanks. The easiest way to simulate this is to make the upper boundary (top surface of the water) a sliding wall. This method has drawbacks, because it is a rigid surface, unlike real air, but Flo++ does not make provision for simulating wind as a second fluid flowing over the first without mixing. Nevertheless, the sliding wall approach can be used to investigate a relative affect. Two simulations were done: one with wind

blowing from the inlet side to the outlet side, and another *vice versa*. The effective velocity of the wind at the surface (*i.e.* the sliding wall's velocity) was specified as 1 m/s in both cases. The effect of a crosswind over the tank (i.e. in the z-direction) could not be simulated with the existing model, because mesh symmetry is used in the code. Due to the presence of the side walls, such a simulation would not be realistic. The results are displayed in figures f7_10 and f7_11. With the wind blowing from the outlet side to the inlets a surface and bottom current flow developed. The bottom current prevented particles from being trapped in the inlet vortices and they followed trajectories parallel to the bottom of the tank and below the upper third of it (figure f7_11). With the wind blowing from the inlet side to the outlets, (figure f7_10) secondary vortices developed in the uppermost left side corner and in the first sump. Particles were also swept upwards towards the short-circuiting (to the outlets) surface current.

Operational experience at Midvaal has shown that wind does indeed have a very significant effect and that the effect corresponds well with the simulation. (Pietersen, 2003.)

7.4 Effect of changes in tank configuration.

Removing the first three rows of sumps:

Because all the simulations done on changes in operational parameters showed that there was significant interaction between the inlet vortices and the sumps directly below it, the effect of the removal of the sumps from the design was modelled. The result is shown in figure f7_12. It is obvious that the sumps have a very significant influence on the inlet zone. Without the first three rows of sumps, the inlet vortex cannot develop and it is flattened into an ellipsoid shape. Despite the apparently reduced complexity of the configuration, flow was less stable, as was shown by an increase of 17.5 % in iterations for the solver.

Addition of a baffle at the inlets:

It is common practice to install a baffle at the inlets to break up the inlet jets. The effect of doing this in the Midvaal tank is shown in figure f7_13. In this specific case it caused the formation of three strong vortices in the inlet zone, causing more

particles to become trapped, especially of smaller diameter. Also, the particles that did escape were swept upwards into a surface current.

If the vortices at the inlet zone encourage further flocculation, the trapping effect will be beneficial.

Changing the position of the baffle, e.g. to right above the middle of the first sump, will change the flow patterns, but will increase turbulence and shear forces, as was observed in the labtank simulations.

Moving the inlets higher on the inlet side:

As was stated previously, the positioning of the inlets in the lower part of the tank causes a left-turning vortex, i.e. an upward flowing one in this case. This is the opposite of the Jönköping and labtank cases, therefore the effect of moving the inlets higher up on the wal was simulated. In the first simulation the lowest row of inlets were moved up to above the higher ones, thus positioning the inlet symmetrically close to both sides of the middle of the inlet side. (Figure f7_14.) For the next simulation, this procedure was repeated, leaving both rows of inlets in the upper third of the inlet side, similar to the labtank. (Figure f7_15.)

The effect on flow patterns and particle trajectories in the inlet zone was dramatic. With the inlets in the middle, the inlet vortex split into two: a weaker one still flowing upwards (left-turning); the stronger one flowing downwards (right-turning). With the inlets in the middle, fewer particles were trapped in the vortices, especially smaller ones. In both cases the particle trajectories to the settling zone are now along the bottom of the tank, ranther than the top.

Figure f7_16 also shows the simulation with inlets at the top, but with a different colour scale range to provide better resolution of detail for the rest of the tank. Because of the higher flow velocities over the sumps in the inlet zone, it is likely that less particles will settle out in these sumps.

Changing the outlet design:

In chapter 5 it was stated that the outlet design appears to have less influence on the hydrodynamics of the tank than normally believed. To investigate this, a radical change in outlet configuration was modelled. The outlet design was changed from outlet channels projecting into the tank from the outlet side to a simple weir-type outlet at the back wall. The results are given in figures f7_17A and f7_17B. The effect on the flow patterns could only be observed if the colour scale range was changed by decreasing the maximum by an order of magnitude (i.e. all flow above 2,829 x 10⁻² is shown as maximum instead of 2,882 x 10⁻¹). This showed that for practical purposes the effect is limited to the outlet zone. A very small effect can be observed in the particle trajectories in the inlet zone and also in the top layer of the settling zone.

The relative effects of changing inlet and outlet configuration simultaneously is shown in figure f7_18. The inlets were positioned at the top and the outlet was again a weir at the back wall. Comparison with figure f7_16 shows that the inlet zone and particle trajectories are unaffected by the changed outlet design.

Summary of results

- As with the simulations of the labtank it was found that the computational grid must be refined at the inlets and the outlets to obtain grid independence and computational stability.
- Unlike the labtank, the solid phase did not affect the flow patterns significantly.
 This is due to the particle concentration being three orders of magnitude lower,
 and to the inlets being situated in the lower half of the tank rather than the upper half.
- Trapping of the particles in the inlet zone by the the vortices caused by the inlet jets were again observed.
- The flow patterns were remarkably stable under a wide variety of operational conditions, e.g. changing particle concentration. or characteristics, water flow rate, water temperature of inlet velocity vectors..

- Water temperature affected the stability of the flow. With increasing temperature, the number of iterations required for convergence increased by 44% when the temperature was increased from 11 to 21 °C.
- Wind was shown tom have a significant effect on flow patterns, corresponding to operational experience at the plant.
- The effect of changes to the tank configuration depended on the type of changes.
 Removing the first three rows of sumps had a very significant influence on both the flow patterns and stability in the tank as a whole. So did moving the inlets upwards. Adding a baffle affected the inlet zone, but not the settling and outlet zones, as was also found in the labtank simulations and experiments.
- As with the labtank, outlet design was found to only affect the outlet zone, not the inlet or settling zones.
- CFD (specifically Flo++) simulations were stable and did yield results in accordance with practical operational experience at the plant, also explaining some observations made, e.g. the clearly demarcated floc blanket in the inlet zone.
 This confirms the realism and dependibility of the technique and demonstrates it usefulness for such investigations.

8. DISCUSSION AND CONCLUSIONS

A. Suitability of CFD for modelling and simulation of rectangular sedimentation tanks as a tool for research, design and development.

The results of the CFD simulations done during this project and reported in literature demonstrates that CFD has reached a level of development in theory, code (algorithms and application packages) and computer hardware where it has become a useful tool for research, design and operation in water technology. It is now possible to use standard software packages and desktop computers to analyse and investigate fairly complex situations in terms of configurations and conditions within reasonable time periods and at lower cost than doing experimental work.

Obviously there are limitations inherent to the technique. In reality, for example, the real size distribution of floc particles is too large to simulate. Also, the flow domain has to be approximated by a finite number of cells of finite volume. This limits the resolution of models. Numerical rounding also also affects accuracy. Nevertheless, it is possible to develop very realistic models. These are models that mimic nature in such a way that the behaviour of the models cannot be distinguished from that of the physical systems they are modelling. Such models can therefore be used with confidence to investigate the characteristics and behaviour of the physical systems, including the effects of changes in or to it.

The realism of the CFD models developed in this project led to valuable insight into the dynamics of the tanks. One example occurred during the investigation of the effect of temperature. It was found that the water temperature did have a significant effect on the numerical behaviour of the models: at the lower temperatures (4 – 15 °C) the models converged much more quickly than at the higher ones (15 – 25 °C). In the case of the labtank, the models ususally did not converge at all at the higher temperatures, but had to be solved as unsteady cases. This was at first thought to be due to numerical reasons – it is an often used trick in CFD modelling to increase the fluid viscosity (i.e. lower temperature) initially to speed up the solution. The physical experiments with the labtank showed it to be due to the physical reality. The physical

system was behaving non-linearly (i.e. chaotically) at the higher temperatures. Hydrodynamic instability rather than numerical instability was causing the nonsteadyness in the numerical model, just as was occurring in the physical labtank. When similar nonsteady behaviour was experienced during the simulations of the Midvaal tanks (e.g. simulating the effect of removing the first three rows of sumps at the inlet side) it was not assumed to be numerical instability, but evaluated as a real physical phenomenon. This is an example where CFD modelling showed that a configuration modification that was intuitively expected to simplify the dynamics of the tank, would instead cause it to become significantly less stable and robust and thus susceptible to changes in operational conditions.

One caveat must be noted: CFD packages are not merely customised combinations of CAD packages with spreadsheets. As with all engineering applications, they are specialized tools that require both a thorough theoretical background and considerable experience of implementing to yield good, reliable results. This expertise is becoming more readily available.

Special aspects and requirements of CFD modelling of sedimentation tanks.

Single and two phase modelling.

The results of the physical experiments and CFD simulations done during this project showed that the presence of the solid phase, i.e. floc particles, in the water affects the dynamics of sedimentation tanks. Therefore two-phase simulation will normally be required to obtain realistic information for design and operational purposes.

To do two-phase modelling the solid phase can be simulated as either another fluid (i.e. the sludge) completely mixed with the water entering the tank, or as discrete solid particles. Both approaches have their own advantages and disadvantages. (See paragraph 3.1.2 for a discussion.) When the project was initiated it was not practically feasible to do two-phase simulations by means of discrete particle tracking, due to hardware constraints. However, the rapid development of computer hardware has now made this a viable option and the consequent realism of the models and the amount of information that can be obtained in this way make it preferable to the scalar (mixed

fluids) approach in many instances. Discrete particle tracking yields more information about the interaction of the water and the particles and insight into the development of the flow patterns than the scalar approach. For instance, particle tracking makes the unsteady nature of the settling of the particles and its effect on the flow (and vice versa) visible. On the other hand, particle tracking is computationally much more intensive and time consuming and is unnecessary if the modeller is not particularly interested in the particle trajectories. It is also almost impossible to use it to calculate solids concentration in the outflow, since one needs a very exact particle size distribution to do so. The scalar approach can do this much easier.

Computational grid development.

The complexity of the computational grid always requires a balance between the resolution required and the computational requirements. In order to obtain meshindependent solutions that are realistic simulations of the physical reality the grid must be as detailed and as fine as possible, but to optimise time frames and hardware requirements as few cells as possible must be used. One method to do this is to make use of symmetry planes to reduce the number of cells needed. Another is to refine the grid in areas where the flow is the most dynamic and make it coarser where it is not. Detailed grids must be developed for inlets and outlets, *i.e.* the grid must be refined in these areas. This will enable the flow to develop (numerically) correctly and realistically in the inlets and outlets themselves, which leads to much less instability in the main area of the tank model. It also provides better resolution. The same should be done for any area with large variations in velocity, e.g. vortices.

When discrete particles (Euler-Lagrange) modelling is used to do two-phase modelling pseudo 2D models (where a slice of only one layer thickness is used) cannot be used. The grid must be more than one cell layer thick for the fluid flow to develop around particles, even though the particles' dimensions are orders of magnitude smaller than that of the cells.

Floc characteristics and simulation of flocs.

Floc characteristics.

It was found that the physical characteristics of the flocs (size, shape, density, concentration and composition) are not such significant parameters in the operation and performance of the tanks as originally assumed.

Floc composition and structure.

In paragraph 2.2.1 the issues involved in floc composition and structure as relevant to modelling of their settling behaviour is discussed. There was very little information related to this for South African water sources available. In order to obtain some, solids present in the local Mooi River in Potchefstroom was flocculated by means of conventional jar tests with different metal hydroxides as coagulants. The flocs formed were observed under an optical microscope to determine their composition in terms of the agglommeration of the different types of solid material suspended in the water. All the flocs observed consisted of a random mixture of the mineral particles, bacteria, algae and diatoms present in the water. The extent of this work is too little to make any definite or final conclusions, but it does show that floc composition will tend to be very variable, depending on seasonal and environmental conditions. This implies that in doing CFD simulations, as well as when designing actual tanks, a large variation in floc particle composition (and therefore size, density and shape) must be considered - at least the possible extremes and typical values, where extremes wil be high mineral content and high microbial content. More research into this aspect is recommended.

Simulation of flocs in the labtank.

Criteria were set for suitable floc simulants (paragraph 4.4.1). A number of substances were tested viz. synthetically prepared flocs, sago grains, maize meal and, finally, ground polystyrene granules. The latter was found to be ideal in all respects and is recommended to any future researchers. The only drawback is that at 1,013 g/cm³ its density is very close to that of water.

Effects of configuration and operational parameters on rectangular sedimentation tank efficiency.

Sedimentation tanks are used primarily to clarify water by letting suspended solids settle out as flocculated particles. The ability of the tanks to do this depends on two aspects: (a) The water flow pattern through the tank, which in turn is determined by the configuration of the tank and by operational parameters (solids concentration, water flow rate and temperature). (b) The settling characteristics of the particles as determined by their shape, size and interaction with the water through drag and buoyancy forces.

Water flow patterns.

Water flow patterns dominated particle settling in determining the dynamics and efficiency of rectangular sedimentation tanks during the labtank experiments and the Flo++ simulations of it, as well as the simulations of the Midvaal tanks. It was observed that the water flow patterns were remarkably stable and robust for any particular configuration. Operational experience at Midvaal confirmed this. With regard to the water flow pattern through tanks it was found that the most important aspect was the **design of the inlets**, especially their placement. Inlets cause high velocity jets of water into the tanks, which in turn cause formation of vortices. These vortices have the largest effect in determining the water flow patterns through the tanks, and also on the particle trajectories by affecting the solids-caused density waterfalls.

Baffles are often used to dissipate kinetic energy and prevent short-circuiting between inlets and outlets. The experiments and CFD simulations done in this investigation showed that as such it was not necressarily effective. Putting baffles at the inlets did not affect flow patterns or particle trajectories through a tank as a whole or at the outlets specifically. Neither did it affect particle settling patterns on the bottom of the labtank. The baffles did have a significant effect on the vortices and particle trajectories directly at the inlets. The vortices were split up into more vortices and the density waterfalls became steeper between the baffles and the inlets. This can have an effect on the flocculation and settling of real floc particles in practice because more vortices and higher velocity gradients at the inlets were observed to capture more of the floc particles and recirculate them. This effectively forms a demarcated sludge bed

or blanket in inlet zone, which can be expected to improve tank efficiency. This is an aspect that can be researched further.

It is especially in optimising inlet and baffle design and operation that CFD can make a valuable contribution. It is ideal to test different configurations and optimize design aspects such as placement and size.

The hydrodynamic parameters were much less important than expected. (I.e. the water flow rate and velocity components in the different axial directions.) The position and relative velocities of the inlet vortices changes to an extent, but the basic flow patterns remained the same. Temperature, which affects water viscosity significantly and density to a small extent, did not affect the flow patterns per se, but did affect the stability of the flow and the settling behaviour of the particles (paragraph 2.2.2).

Outlet configuration is generally thought to influence the flow significantly due to short-circuiting, but was found to have only minor effects on flow patterns and particle trajectories in the physical labtank, as well as on the Flo++ models of the labtank and the Midvaal tank. Only minor differences were observed in flow patterns and particle trajectories in the inlet and settling zones, whether the outlets were in the form of systems of distributed outlet channels, or overflow weirs at the back of the tank, or even merely a holes in the back walls of the tanks. The results of the experiments and simulations of the labtank and full-scale plants in this project showed that the tank space in the outlet zone (the volume of the tanks in the vicinity of the outlets) is mostly inactive in terms of flow - all the dynamic changes occur at the volume in the vicinity of the inlet (inlet zone). Physical changes to the outlets of the labtank and simulated changes in the outlets of the labtank as well as full-scale plants showed either no or negligible effect on the flow patterns through the tanks. These changes consisted of changing the number of holes in the outlet channels, and even removing the outlet changels altogether, leaving only one large hole or a number of smaller holes in the outlet wall side. Doing this did affect the numerical stability of themodels, but not of the final flow patterns. Simulations with simplified outlets, e.g. simple outlet holes in the wall, was more unstable than ones that had a grid structure for flow to develop in the outlets, e.g. channels with holes.

The presence of the settling particles themselves also affected the flow dynamics. Due to their interaction with the water through drag and buoyancy, they cause the development of a density waterfall in the inlet zone. The extent to which this happened was dependent on the concentration of the particles. Without particles in the inflow streams the simulations and labtank model experiments invariably developed direct shortcuts between the inlets and the outlets. With particles, the flow patterns were more complex because the particle-induced density waterfalls interacted with the inlet vortices.

Floc particle settling.

As far as floc particle settling behaviour is concerned, the water flow patterns in the tank had the most significant effect. This was expected, because the conventional design approach is based on this assumption. The effect of the interaction between the settling particles and the water flow patterns on the dynamics of the tanks, as discussed previously, mostly stems from the development of **density waterfalls**. The density effect is a well-known phenomenon, but is normally considered in relation to water temperature. Its development through a diffuse, discrete and mixed solid phase is much less studied and understood and cannot be predicted intuitively or qualitatively in design. Therefore this is another area where CFD is a powerful tool yielding very useful information before construction.

Water **temperature** did affect tank efficiency in the physical labtank to an extent which is usually not considered in the design of the tanks. The increased viscosity and density of water at the lower end in the normal operational temperature range of 10 to $25\,^{\circ}\text{C}$ caused significantly larger fractions and sizes of the particles to be washed out of the tank via the outlets. The Flo++ models of the labtank and Midvaal tank also showed an effect on the particles, but very much less so than in the case of the physical tank. However, the water temperature did have a significant effect on the numerical behaviour of the models. At the lower temperatures $(4-15\,^{\circ}\text{C})$ the models converged much more quickly than at the higher ones $(15-25\,^{\circ}\text{C})$. In the case of the labtank, the CFD models ususally did not converge at all at the higher temperatures, but could only be solved as unsteady cases. Again, it is an open question for further research whether this instability is due to numerical or physical reasons, or both.

Theoretical calculations confirm that the temperature effect should be significant, especially for particles with density close to that of water. This is due to the increased drag (because of increased viscosity) and increased bouyancy (due to increased density) forces on the particles at the lower water temperature (paragraph 2.2.2).

E. Conclusions in respect of design of rectangular sedimentation tanks.

The conventional approach described in the standard handbooks and used during the twentieth century served well. However, to some extent this was due more to overdesign and ad hoc implementation of measures and modifications based on experience than to real understanding of the actual tank dynamics. The conventional approach is based on assumptions that are oversimplifications of the real processes and mechanisms involved in effective operation of the tanks. Raw water quality in Southern Africa and other subtropical regions is extremely variable due to the effects of droughts, floods, population increase and cultural activities (agriculture, mining, industry and recreation). Economics, increasing limited availability of water and environmental responsibility requires optimization of design to have robust and stable operation under divergent conditions. As in everything else in engineering, the technology has advanced; not making use of improved design tools and techniques cannot be justified. The conventional method is still valuable as a tool for the first stage of tank design to obtain general conceptual information, but such a first conventional design should then be subjected to a rigorous CFD analysis of the its configuration and of the effect of changes in operational parameters. At the least such an analysis to assess the suitability of a design should consider extreme as well as typical operating conditions i.r.o. water flow rate, water temperature and particle concentration, size and density. Inlet designs at least should also be checked by means of CFD simulations to determine the actual flow patterns that will develop in practice under the different conditions, as well as their stability.

Overdesign is not only wasteful, but can actually be detrimental. To what extent does overdesign cause ineffective clarification, because the clarified water in the vicinity of the outlets is an ideal medium for microbial (especially algal) regrowth? This is known to occur. It can be investigated by taking samples of flocs in various zones of

tanks and determining not only their composition, but also their structure and physical characteristics like density and shape (sphericity and fractal dimension).

Another question for further research related to design also comes out of this project: Modelling of the full-scale plants showed that the inlet vortices and density waterfalls are the predominant dynamic characteristics. The high-velocity vortices in the inlet zones trap particles, effectively forming sludge blankets where they can flocculate further, or simply recirculate until they move into a lower velocity region from which they can settle out. To what extent is this mechanism an effective part of the clarification process in practice? Could its effect be enhanced by increasing the intensity of the density waterfall, e.g. by dosing flocculation aids like kaolin or bentonite to increase the density of the flocs? It is possible that the vortices perform much of the work ascribed to the flocculation channels and contribute to the sweep-floc action of flocculant aids. This can be investigated by comparing floc size distributions at the end of flocculation channels with those in inlet zones.

BIBLIOGRAPHY

ADDISON P.S., 1997. Fractals and chaos. An illustrated course. Institute of Physics Publishing, Bristol and Philadelphia. 256p.

BROUCKAERT CJ, PRYOR M, BROUCKAERT BM AND BUCKLEY CA. 2000.

A computational fluid dynamic study of an ozone contactor. WISA Conference, Sun City, South Africa.

CHEN W-J (1998) Effects of surface charge and shear during orthokinetic flocculation on the adsorption and sedimentation of kaolin suspensions in polyelectrolyte solutions. Separation Science and Technology. 33(4), pp 569-590.

CORNELISSEN A, BURNETT MG, McCALL RD and GODDARD DT (1997) The structure of hydrous flocs prepared by batch and continuous flow water treatment systems and obtained by optical, electron and atomic force microscopy. Wat. Sci. Tech. Vol. 36, No. 4, pp 41-48.

CORNELISSEN A, BURNETT MG, McCALL RD & GODDARD DT (1997). The structure of hydrous flocs prepared by batch and continuous flow water treatment systems and obtained by optical, electron and atomic force microscopy.

Wat.Sci.Tech. Vol. 36, No 4, pp. 41-48.

DU TOIT, C.G., (2000) Personal communication

DU TOIT CG and LEMMER TN (2000) The application of computational fluid dynamics in the design and operation of rectangular sedimentation tanks in potable water treatment. Presented at WISA 2000 conference, Sun City, South Africa, 28 May – 1 June 2000

ELMALEH S and JABBOURI A (1991) Flocculation energy requirement. Wat. Res. Vol 25, No 8, pp 939-943. FERZIGER, J.H. and PERIC, M., (1996) Computational Methods for Fluid Dynamics, Springer-Verlag Berlin-Heidelberg.

HAARHOFF J, VAN BEEK JC and VAN ZYL HJ (1996) Practical application of the Argaman-Kaufman flocculation model. Paper presented at the 1996 WISA conference, South Africa, 8pp.

LARSEN P 1977. On the hydraulics of rectangular settling basisns, Lund: Lund University. 170p. (Lund Institute of Technology (Sweden) Report no 1001)

LE GRANGE, L.A., (2000) Personal communication

LE GRANGE, L.A., (1994) User Manual for FLO++, Potchefstroom (Unpublished)

LEMMER, T.N. (2000) Personal communication

LEONARD, B.P. (1979) A stable and accurate convective modelling procedure based on quadratic interpolation. Computational Methods Applied Mechanical Engineering 19 59-98

LOGAN BE and KILPS JR (1995) Fractal dimension s of aggregates formed in different fluid mechanical environments. Wat. Res. Vol. 29, No 2, pp 443-453.

LOGAN BE & KELPS JR (1995). Fractal dimension of aggregates formed in different fluid mechanical environments. Wat. Res. Vol. 29, No. 2, pp 443-453.

McCORQUODALE, J.A., (1997) Hydrodynamic modelling. Secondary Settling Tanks: Theory. Modelling. Design and Operation; IAWQ Scientific and Technical Report 6, 105-145

NAKAMURA T, ADACHI Y & SUZUKI M (1993). Flotation and sedimentation of a single microcystis floc collected from surface bloom. Wat. Res. Vol.27, No. 6,pp 979-983. PATANKAR, S.V., (1980) Numerical heat transfer and fluid flow. McGraw-Hill, New York

PATRY, G.G. AND TAKACS, I., (1992) A dynamic model of the clarificationthickening process. Water Research, 26(4) 473-479

PEAVY HS, ROWE DR & TCHOBANOGLOUS G, 1985. Environmental engineering. International edition, McGraw-Hill Book Co. Singapore. 699 pp.

PIETERSE AJH & CLOOT A (1997). Algal cells and coagulation, flocculation and sedimentation processes. Wat. Sci. Tech. Vol 36, No4 pp111-118.

PIETERSE AJH and CLOOT A (1997) Algal cells and coagulation, flocculation and sedimentation processes. Wat.Sci.Tech. Vol 36, No 4 pp 111-118.

SHAW CT, 1992. Using computational fluid dynamics. Hertfordshire: Prentice Hall International (UK) Ltd. 251p.

STANDER, G.J. 1995. The socio-economic value of water as a key factor in water quality control in a geographic area. *Chemical Processing SA*, August: 10-13.

STOVIN, V.R. AND SAUL, A.J., (1998) A Computational fluid dynamics (CFD) particle tracking approach to efficiency prediction. Water Science and Technology 37, 285-293

TAKACS I, PATRY GG & NOLASCO D, 1991. A dynamic model of the clarification-thickening process. Wat. Res., pp 1263-1271.

TCHOBANOGLOUS G & BURTON FL (1991) [Metcalf & Eddy, Inc] Wastewater engineering. Treatment, disposal, reuse. 3rd edition. McGraw-Hill, Singapore.1334 pp

VAN DER WALT J.J. (1994) Numerical modelling of two phase flow in process tanks. Potchefstroom: PU for CHE. (Dissertation for M.Eng.) 172 pp. VERSTEEG HK & MALALASEKERA W, 1995. An introduction to computational fluid dynamics – the finite volume method. Essex: Longman Scientific & Technical. 257p.

WEAST R.C. (1979) CRC Handbook of physics and chemistry. 60th edition. CRC Press, Inc. Boca Raton, Florida.

ZHOU. S. & McCORQUODALE J.A. (1992) Modelling of rectangular settling tanks, Journal of Hydraulic Engineering 118(10) 1391-1405

APPENDIX A

Geometric description of the Labtank.

The outlet side of the perspex structure of the Labtank is shown in Figure A1. The inlet side is described in Figure A2.

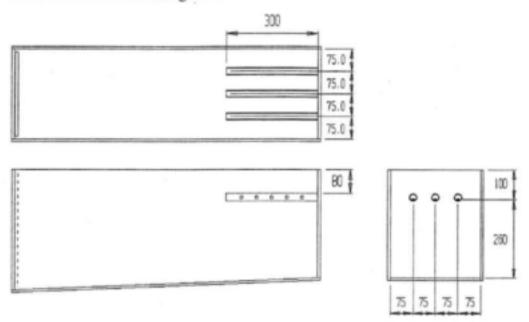


Figure A1 Top, side and outlet view of the Labtank.

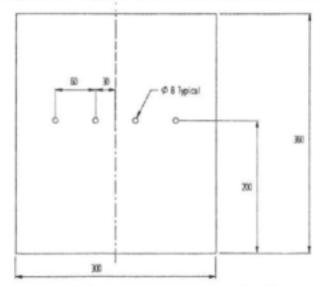


Figure A2 Inlet side view of Labtank. The shown inlets of 8mm replaced inlets of 20 mm diameter. Inlets are equally spaced 60mm between centres around the centreline of the tank.

APPENDIX B

Development of the water delivery system

In order to simulate the flow in the Labtank numerically, conditions have to be as close to ideal as possible. This poses strict requirements on the water delivery system to the Labtank.

Requirements on the delivery system:

- 1. Flow distribution between inlet holes have to be equal
- Volume flow rate must be measured accurately over the course of an experiment.
- 3. Inflow to the tank has to be free of large air bubbles.

The final experimental layout for the delivery system is shown in Figure B1

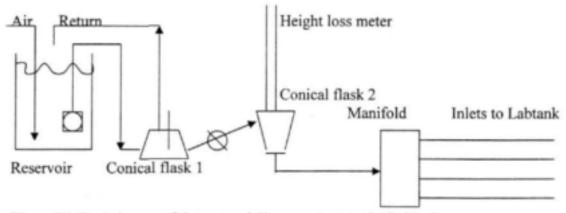
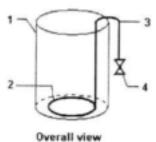


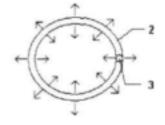
Figure B1 Basic layout of the water delivery system to the Labtank

This system functions as follows:

100 liter Reservoir tank

Washed maize meal is used to simulate flocs. Compressed air is bubbled through the reservoir to keep the flocs in suspension. A floating centrifugal pump pumps water to conical flask 1. The setup of the air supply system is explained in Figure B2. The pump stalls when air is sucked in, but the inlet concentration of flocs to the pump must remain constant. These opposite requirements are compromised by attaching a bubble deflector to the pump's bottom, and an elbow to the suction pipe. Figure B3 displays the arrangement.

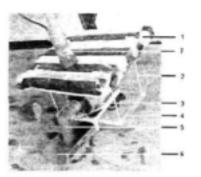




- 1. Reservoir
- 2. Holed air distribution tube
- 3. Air delivery hose
- 4. Regulating valve

Overall view Top view of air hose

Figure B2 Setup of pressurised air stirring apparatus (Used with permission B.G. van Duuren)



- 1. Pump float
- 2. Mounting wire
- 3. Pump
- 4. Bottom plate
- 5. Elbow inlet
- 6. Bubble deflector
- Pump outlet

Figure B3 Pump system (Used with permission B.G. van Duuren)

Conical flask 1

The regulating valve after flask 1 forces excess water to flow via the return pipe to the reservoir tank. Inlet flow velocity is high enough that adequate turbulence exists to keep flocs from settling.

The inlet and Labtank outlet is situated at the bottom of the flask, with the return outlet at the top, so that any air bubbles sucked in by the pump is returned. This flask also contains a thermometer.

Conical flask 2/Volume flow meter

This flask is used to provide a flow stagnation condition to measure the total height difference between the Labtank surface and the delivery system. Because height difference is related to volume flow rate, this height meter can be calibrated to indicate volume flow rate.

This flask has to stand upside-down, with its outlet at the bottom, otherwise flocs settle and the solids concentration of the delivery water doesn't remain constant. Figure B4 shows how the height meter looks from nearby.

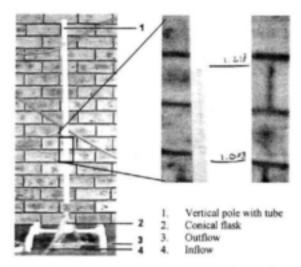


Figure B4 Flow rate measurement tool. The flask depicted is from the previous configuration. (Used with permission B.G. van Duuren)

The meter can be calibrated and a curve is fitted for very accurate flow rate measurements. An example of a flow rate/height curve is shown in Figure B5.

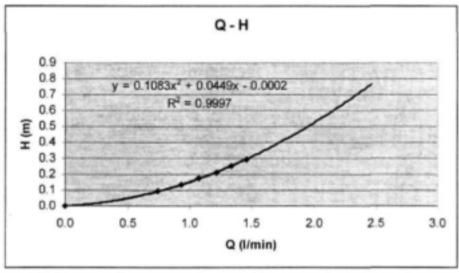


Figure B5 Diagram of height loss as function of flow rate in the sludge supply system.

Manifold

A compact water division manifold was made to replace a bulky, tee-junction dividing system. Flow channels were milled into a block of perspex, with the plastic delivery pipes clamped between the bottom flow canal block, and the top closing block. A water-tight seal is obtained by putting vaseline on all surfaces. See Figure B2

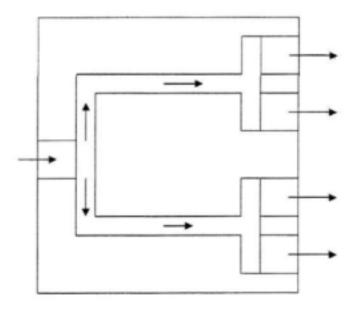
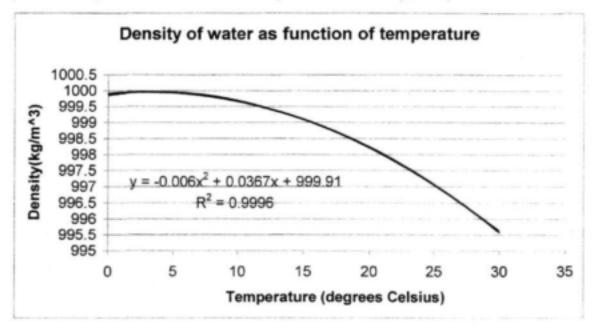


Figure B.2 Schematic diagram of the flow distribution manifold

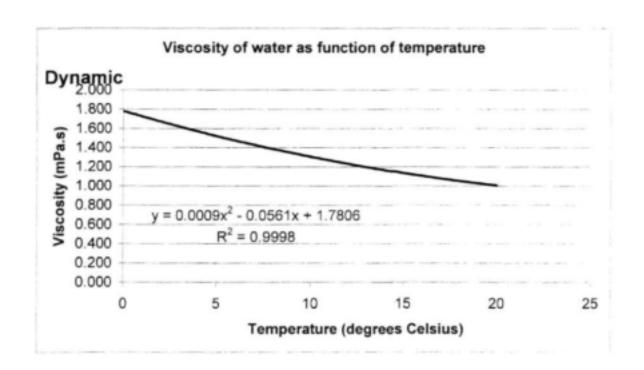
APPENDIX C

Properties of water

(From Weast, R.C. CRC Handbook of Physics and Chemistry, 1985)



Deg.C		kg/m^3
	0	999.8395
	1	999.8985
	2	999.9399
	3	999.9642
		999.972
	5	999.9638
	6	999.9402
	7	999.9015
	8	999.8482
	9	999.7808
	10	999.6996
	11	999.6051
	12	999.4974
	13	999.3771
	14	999.2444
	15	999.0996
	16	998.943
	17	998.7749
	18	998.5956
	19	998.4052
	20	998.2041
	21	998.0347
	22	
	23	997.5800
	24	
	25	997.0800



degrees C	Pa.s x 10e-3
0	1.787
1	1.728
2	1.671
3	1.618
5	1.567
	1.518
6	1.472
7	1.428
8	1.386
9	1.346
10	1.307
11	1.270
12	1.235
13	1.202
14	1.169
15	1.139
16	1.109
17	1.081
18	1.053
19	1.027
20	1.002
21	0.9994
22	
23	0.9664
24	
25	0.9406

APPENDIX D

Measurement of maize meal density

Procedure

- Calibrate measuring beaker.
 - Fill the beaker with 100ml of water by using a burette.
 - Clearly mark the water level at 100ml (V_0)
- Empty and dry the beaker. Then weigh the beaker. (Wb)
- Fill the beaker with less than 100 ml maize meal
 Weigh the beaker containing the meal. (W_{bm})
- Add water to the meal in the beaker to the marked level of 100ml by using a burette. Measure the amount of water added to reach 100ml. This volume is called the filling volume. (V_{fill})
 - Stir the meal so that all air bubbles can escape. After all the air has been removed, ensure that the water level is again at 100ml.

Calculation:

Density of meal = $(W_{bm} - W_b)/(V_0 - V_{fill})$

Result of measurement done on 22/8/2000

$$W_{bm} = 153.02g$$

$$W_b = 104.12g$$

$$V_0 = 0.1001$$

$$V_{fill} = 0.06541$$

Density of maize meal =
$$(W_{bm} - W_b)/(V_0 - V_{fill})$$

= 1410 kg/m^3

APPENDIX E

Derivations and calculations

1. Calculation of particle mass injection rate

Nomenclature

C_{uv}	M/L^3	Inlet solids concentration
d	L	Mean particle diameter
m	M/T	Particle mass injection rate
N	-	Number of parcels in numerical simulation
n	T^I	True number of particles injected into tank per second
n/N	T^{I}	Number of particles per parcel
V_p	L^3	Particle volume
$\rho_{_{p}}$	M/L^3	True density of flocs (particles) in water

$$m = n\rho_{p}V$$

$$m = N \cdot \frac{n}{N} \cdot \rho_{p} \frac{\pi d^{3}}{6}$$

$$\therefore \frac{n}{N} = \frac{6m}{N\rho_{p}\pi d^{3}} = \frac{qC_{in}}{60000} \cdot \frac{6}{N\rho_{p}\pi d^{3}}$$

$$\frac{n}{N} = \frac{q[l/\min]C_{in}[g/l]}{10000\pi N\rho_{p}d^{3}}$$

The formula above was deducted in order to relate solids concentration, volume flow rate and particle characteristics with the number of particles employed in the numerical model.

2. Computation of spherical particle settling velocity

As stated in Peavy et al. (1985) the Stokes equation in valid only for laminar flow, i.e. when the Reynolds number Re < 1.

The Stokes equation states:

$$v_0 = \frac{g(\rho_p - \rho_w)d^2}{18\mu}$$
 (F.1)

$$Re = \frac{\rho_* v_0 d}{\mu}$$

Substitution of the Stokes equation in the Reynolds number gives:

$$1 > \frac{\rho_* g d^3 (\rho_p - \rho_*)}{18 \mu^2}$$

Rearrangement gives the following criterion for validity of the Stokes equation:

$$\frac{18\mu^2}{g\rho_w} > d^3(\rho_p - \rho_w)$$
 (F.2)

If the above criterion is satisfied, the Stokes equation can be used to determine the settling velocity of the particle. Should the criterion not be satisfied, flow around a particle will be turbulent, and Re > 1.

For a turbulent flow condition, the coefficient of drag $C_d = 0.4$

At settling velocity, buoyant force equals drag force, therefore:

$$(\rho_F - \rho_w)g \times \frac{\pi d^3}{6} = 0.4 \times \frac{\pi d^2}{4} \times \frac{\rho_w v_0^2}{2}$$

Rearrangement gives:

$$v_0^2 = \frac{(\rho_p - \rho_w)dg}{\rho_w} \times \frac{8}{6 \times 0.4}$$

$$\therefore \qquad (F.3)$$

$$v_0 = \sqrt{\frac{(\rho_p - \rho_w)dg}{0.3\rho_w}}$$

Procedure for calculating settling velocity

The following procedure can be established for computing the settling velocity of a spherical particle:

- Determine whether the Stokes criterion (Eq. F.2) is satisfied.
- If it is satisfied, use the Stokes equation (Eq. F.1).
- If not, use the turbulent settling velocity equation (Eq. F.3).

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JJ Smit and GP Greyvenstein

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EIS studies concentrated on the development of an electrolytic cell to generate impedance spectral data, used for static modelling of a membrane in an electrolyte as a resistancecapacitance electrical circuit.

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