Docotrall Thesis

Particle separation processes with emphasis on blood separation

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Particle separation processes with emphasis on blood separation

A dissertation submitted to the

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Zurich, 2005
E fu così che una vacca sacra dell’India che non era mai stata nella Palestina passando di fronte a un ristorante italiano riconobbe da fuori la sua vecchia cugina che lavorava come bistecca alla fiorentina in un ristorante italiano in Palestina e le chiese la strada per andare a trovare dove la terra si incrocia col cielo e col mare qualcuno le disse viaggiare è importante ma il posto che cerchi non è molto distante da dove ti trovi e da dove stai andando unisciti a noi che ci stiamo arrivando e se nel cammino noi poi invecchieremo ci saranno degli altri poi altri poi ancora fin quando qualcuno nell’anno del dunque sarà in nessun posto e sarà pure ovunque

Jovanotti
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Sandro De Gruttola
Summary

Needs for separating mixtures are pervasive in various industries and daily applications. With increased attention in recent years to prevent pollution of the environment and recovering new products, as well by needs of many other industries, as in the medical field, the variety of particle-fluid separation processes to be accomplished has widened. In addition, the arsenal of available methods of separation and means of implementing particular methods of separation has become more extensive. Hence there has been a growing need for practicing engineers and scientists to develop an understanding of the capabilities of different methods of separation and different separation equipment on a comparative basis.

The scope of this work is to develop a numerical method to calculate the behaviour of particle separation processes focusing on the blood separation. This numerical model is then implemented and simulations for different separation processes are performed. The basic idea of this method is to simulate solid particles moving in a fluid. These particles settle depending on the flow field and fluid properties. The development of the computational model and code occur within three steps. To this end, different separation scenarios and fluid behaviour have been modelled: Separation due to gravity and centrifugal force, and separation within a constant or variable (non-Newtonian) viscosity fluid.

The expression apheresis comes from the Greek language and means ‘to subtract’. It may be described as a process by which blood being removed from a subject is continuously separated into its components, usually to allow a desired component (or components) to be retained while the remainder is returned to the subject. This is done for different reasons. Blood cells survive longer outside the body, if they are separated and stored in a proper manner. Another use of apheresis is for therapeutic reasons. Therapeutic apheresis is used in the treatment of a variety of diseases and syndromes. The main idea is to subtract a sick or overnumbered part of blood cells and then give the healthy part back to the patient, or to replace some blood cells with cells of a healthy donor. To exemplify patients with acute leukaemia with hyperleukocytosis (overproduction of white blood cells) are exposed to a high risk of fatal cerebrovascular haemorrhage. Thus cytapheresis (extracting white blood cells) is applied on these patients to avoid cerebral apoplexy (stroke). The blood separation occurs under the acceleration in a rotational field. The centrifugal force is large enough to separate the discrete blood components on the basis of differing densities, while overcoming the force of diffusion in the cellular-plasma suspension of blood.

Computational fluid dynamics (CFD) is a tool used to study fluid flow. More specifically, CFD is a numerical methodology in which the fluid flow governing partial differential equations are approximated through discretization into algebraic equations, and these equations are solved using iterative techniques with the calculating power of a computer. CFD has found its way into all branches of engineering and science. Optimization by such techniques can enhance performance, reduce concept-to-prototype time, produce large savings in equipment and energy costs as well as reduce environmental impact. Many models exist to calculate the fluid flow. For the separation simulations a hybrid (Lagrangian-Eulerian) method has been used. Within the Eulerian method the flow field of is calculated. Once the flow field is calculated, the particle path is evaluated. Dependent on the particle concentration in the fluid and the fluid properties, a back-coupling of the particle flow and flow field
calculation takes place. The flow field is then re-calculated for the next time step. This process continues, until the flow reaches quasi steady state behaviour.

A new geometry of sedimentation basins having similar physics with blood separation has also been investigated. Water with a low concentration of glass particles is flowing into a sedimentation basin. The separation occurs due to gravity. Due to the low particle concentration, the water flow field is not affected by the particle movement. Hence, the water flow field is calculated first. Then the particle flow is calculated over different time steps using the flow field and geometry information. The sedimentation efficiency of the new basins, regarding different particle sizes, was investigated. The sedimentation efficiencies are lower than in already existing systems. Hence, the new system is not an improvement compared with existing devices. Within this part of the dissertation a stable particle integration scheme for this application was implemented.

A two dimensional Newtonian transient model of the apheresis process is implemented. The blood cells, which are modeled as rigid spheres, are separated from the plasma due to centrifugal force. The process is modeled using a hybrid method. First the blood flow field is calculated. Once it converges, the particles displacement at given time step are evaluated. After all particles have moved, the density distribution in the separator is calculated, due to local blood cell concentration. In the next time step the flow field is calculated with the new density distribution. The entire calculation process stops when a quasi steady state is reached. The simulations show good agreement with the experimental results. They exhibit a complete separation of plasma and red blood cells, as well as nearly complete separation of red blood cells and platelets. The white blood cells build clusters in the low concentration cell bed.

The last part of this work is a non-Newtonian model of apheresis. The computational scheme is the same as for the Newtonian model. The main difference is that viscosity changes during the process. Viscosity is calculated using two models based on Vand’s viscosity formulation. Simulations for different geometry lengths and different inlet hematocrits are performed. The results are more accurate than those of the Newtonian model, due to the variable viscosity consideration. Thus viscosity change plays an important role in the separation process. A longer separator improves the separation efficiency, while an increasing inlet hematocrit leads to lower separation efficiencies. The calculated shear stress values are very similar for all simulations. The shear stress remains below critical values, and, consequently, no haemolysis takes place.

Recapitulating, specific separation processes have been modeled and a CFD model, which can simulate these processes, has been developed. These processes are simple gravity sedimentation to centrifugal non-Newtonian blood separation.
Zusammenfassung


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1. Introduction

1.1. Historical background

For thousands of years, the human body was a mystery to the world of science. Indeed, cultures across the globe employed various forms of observation, experience, ritual, intuition, and other methods to combat illness. Nowhere was this more apparent than in the understanding of blood and the circulation systems.

Already ancient cultures believed that blood had an important role in our lives. The Egyptians used ca. 2500 B.C. bleeding to treat patients. A tomb illustration in Memphis, Egypt, depicts a patient being bled from the foot and neck. For the ancient Chinese cultures around 1000 B.C., the soul was contained in the blood [1, 2].

As well the ancient Greeks were concerned about blood and the circulation. Alcmaeon (500 B.C.) of Croton observes that arteries and veins are dissimilar. Hippocrates (400 B.C.), the pre-eminent physician of antiquity, postulates that the body is comprised of four humours and their imbalance caused disease. In addition to humour theory, Hippocrates and his followers set forth tenets that form the basis of much of Western medicine: disease results from natural as opposed to magical causes, patients should be observed and symptoms of disease should be noted, and physicians should adhere to a strict ethical code of conduct [3]. Aristotle (350 B.C.) believed that the heart was the central organ of the body and therefore the seat of the soul. He conducted dissections of many different animals and described their anatomical structures. Based on his observations, Aristotle presumed the heart is a three-chambered organ, even in humans.

Through his studies of anatomy, successful treatment of patients, and voluminous writings on medicine and the philosophy of medicine, Claudius Galenus (130-200 CE), known as Galen, became one of the most important physicians in history, second only to Hippocrates in influence. Dissecting and experimenting on animals, he proved that arteries contain blood, but also suggested that the system of arteries and veins are completely distinct, and blood forms in the liver. His ideas, not all of which are correct, formed the core of the medical canon for centuries [3].
First steps in blood transfusion were made in the 15th century. In 1492, Pope Innocent VIII of Rome had an apoplectic stroke, became weak and went into a coma. His physician advised a blood transfusion as a therapeutic measure for the Pope's illness. Employing crude methods, the Pope did not benefit and died by the end of that year. It was widely believed in the middle age that the drinking of human blood was a method where a person's health could be restored. This was the first reported transfusion in history [2].

In 1628 the British physician William Harvey published his work in which he explained that blood circulates within the body and is pumped by the heart.

The development of the microscope helped the understanding of blood and its circulation substantially [4]. Thirty years after Harvey, Jan Swammerdam, a 21-year-old Dutch microscopist, is believed to be the first person to observe and describe red blood cells in the year 1658. At nearly the same time, the Italian anatomist Marcello Malpighi observed the capillary system, the network of fine vessels that connect the arteries and the veins, using a rudimentary microscope. The red blood cells were described more precisely in 1667 by Anton van Leeuwenhoek, a Dutch microscopist, who unaware of the work of Swammerdam and Malpighi, described the size of the red blood cells "25,000 times smaller than a fine grain of sand" [2].

The eminent British obstetrician and physiologist James Blundell performed in 1818 the first recorded human-to-human blood transfusion. Using a syringe, he injected a patient suffering from internal bleeding with 12 to 14 ounces of blood from several donors. The patient died after initially showing improvement [5].

Sir William Osler observed that small cell fragments from the bone marrow make up the bulk of clots formed in blood vessels; these cell fragments will come to be called platelets. He discovered them in the year 1874 [6].

The Austrian physician Karl Landsteiner published in 1901 a paper detailing his discovery of the three main human blood groups A, B, and C, which he later changes to O. This helps the transfusion of blood to be successful [7].

Almost simultaneously, researchers Albert Hustin of Brussels and Luis Agote of Buenos Aires discovered in the 1914 that adding sodium citrate to blood will prevent it from clotting. One year later, Dr. Richard Weil determines that citrated blood can be refrigerated and stored for a few days and then successfully transfused.
While serving in the U.S. Army, Dr. Oswald Robertson, collects and stores type O blood, with citrate-glucose solution, in advance of the arrival of casualties during the Battle of Cambrai in World War I, thereby establishing the first blood depot [2].

From the First to the Second World War, scientists and physicians inspired rapid progress in the large-scale storage and use of blood. War was not an incidental factor to these developments, as it created unprecedented demand for the life-saving fluid. Much as the Spanish Civil War was a prelude to World War II, and blood was first transported to the front lines of battle in Spain. By the time war had spread through Europe, the Allied forces were aided by a well-organized blood supply.

In 1940, Drs. Karl Landsteiner and Alex Wiener discover the Rh blood group, through experiments with the red blood cells of Rhesus monkeys, and identify the antibody found by Levine and Steston to be anti-Rh [7, 8].

A plasma shortage in Britain during World War II prompted the U.S. to organize the Plasma of Britain campaign, run by Dr. Charles Drew from a central laboratory at Presbyterian Hospital in New York. Building on techniques he had already developed to separate and preserve blood plasma, which he found to be a viable substitute for whole blood, Dr. Drew devised a modern and highly sterile system to process, test, and store plasma for shipment overseas by the Red Cross [2].

Dr. Carl W. Walter developed in 1948 a plastic bag for the collection of blood and brought a big change in the history of blood processing and storage. Prior to this, glass bottles were used to store blood, but their fragility and susceptibility to contamination prompted him to devise a stronger and more portable container using plastic, which revolutionized blood collection [8].

In the 1950s, three main discoveries and newly developed processes had a great impact on the transfusion and processing of blood. The development of the refrigerated centrifuge began to further expedite blood component therapy. Products made from blood plasma were developed to treat diseases such as chicken pox. As well the human Leukocyte Antigen System (LAS) was developed. The human leukocyte antigen system is the major histocompatibility complex antigen system in humans. The proteins on the outer part of body cells that are unique to that person. Any cell displaying that person's LAS type belongs to that person. When a foreign pathogen enters the body, specific cells called antigen presenting cells grab that pathogen inside. Proteins from that pathogen are chewed up into small pieces and
loaded onto LAS antigens. Due to these different developments in 1960 Solomon [9] and Fahey [10] reported the first therapeutic plasmapheresis procedure. In the 1960s the role of platelet concentrates in reducing mortality from hemorrhage in cancer patients was recognized. Plasmapheresis was introduced as a means of collecting plasma for fractionation. In 1969 S. Murphy and F. Gardner demonstrated the feasibility of storing platelets at room temperature, which revolutionized platelet transfusion therapy [11, 12].

From the beginning of the 1970s on, apheresis was not only used for the blood storage, but it was used to extract one cellular component, returning the rest of the blood to the donor. Therefore technology made progress and different models were developed. With the discovery of new illnesses there is still much to do in the development of blood separators.

1.2. What is apheresis

In 1914 demonstrated the feasibility of removing large quantities of plasma from a dog by a process called plasmapheresis [13]. The expression apheresis comes from the Greek language (αφαίρεσις) and means to subtract or eliminate. It may be described as a process by which blood being removed from a subject is continuously separated into components parts, usually to allow a desired component (or components) to be retained while the remainder is returned to the subject. Apheresis is categorized in two different types: apheresis for donation and therapeutical apheresis.

1.2.1. Donation

During early years of blood banking and transfusion, whole blood was collected into bottles and there was little opportunity to manipulate the blood. Often glass bottles, where the blood was collected and transported, burst. As well glass didn’t support the loads during the cell separation. With the advent of plastic bags for blood collection, it became possible to separate blood into its components. Plastic bags made it possible to collect larger amount of blood, because it portability is very good. This coincided with the recognition that many diseases manifest themselves in patients by lacking only a portion or component of the blood or having more deficiencies of some components than to others. These patients needed transfusion of only specific blood components from healthy donors. Thus donated blood was separated into its component to satisfy the needs of the patients.
If platelets are stored at an appropriate temperature (between 22°C and 37°C), in plastic bags, they have a survival time of eight days, and have a quite satisfactory in-vivo viability [14-18]. If they are stored at temperatures under 22°C their survival time decreases, e.g. if stored at 13°C the survival time is around four days [11]. Compared with the storage time of the RBCs, their survival time is very short. RBCs are produced in the bone marrow and can be stored at 1-6°C for up to 42 days [19] and 10 years if frozen. As well the plasma can be frozen and stored over a longer time. Thus it is an advantage to separate donated blood.

1.2.2. Therapeutic apheresis

Therapeutic apheresis is used in the treatment of a variety of diseases and syndromes. The main idea is to subtract a sick or over numbered part of blood cells and then give the healthy part back to the patient, or to exchange some blood cells with cells of a healthy donor. The Gillian-Barré syndrome is an acute progressive illness affecting the peripheral nervous system. It provokes paresthesias in the extremities and weakness in the respiratory system. About one quarter of the patients remain ambulatory, while at least one quarter need mechanical ventilation at some point. The mortality rate is about 5% [20, 21]. Therapeutical plasma exchange (TPE), the exchange the patients plasma with plasma of a healthy donor, was the first treatment shown favorable to alter the course of the disease. Controlled trials were organized and these trials documented the effectiveness of TPE in shortening recovery time and reducing disability [22-24].

Patients with acute leukemia with hyperleukocytosis are exposed to a high risk of fatal cerebrovascular hemorrhage [25]. Thus cytapheresis (separation of WBCs) is applied on these patients to avoid cerebral apoplexy (stroke). That means that from the patients blood leukocytes are withdrawn and the rest of the blood is restituted. The early mortality forms the basis for performing cytapheresis in symptomatic patients. Ventura[26], Hug [27] and Cuttner [28] showed the benefit of this therapy and the prevention of early death.

The American Society of Blood Banks (AABB) and the American Society for Apheresis (ASFA) have each published similar guidelines and recommendations for use of apheresis therapy [29, 30]. Within Table 1.1 some of these diseases, which are treated with therapeutical apheresis, listed and categorized.
<table>
<thead>
<tr>
<th>Disorder</th>
<th>Procedure</th>
<th>AABB Category</th>
<th>ASFA Category</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABO-incompatible organ or marrow transplant</td>
<td>TPE</td>
<td>III</td>
<td>II</td>
</tr>
<tr>
<td>AIDS</td>
<td>TPE</td>
<td>IV</td>
<td>NR</td>
</tr>
<tr>
<td>Aplastic anemia</td>
<td>TPE</td>
<td>IV</td>
<td>III</td>
</tr>
<tr>
<td>Chronic inflammatory demyelinating polyneuropathy (CIDP)</td>
<td>TPE</td>
<td>I</td>
<td>I</td>
</tr>
<tr>
<td>Coagulation factor inhibitors</td>
<td>TPE</td>
<td>III</td>
<td>II</td>
</tr>
<tr>
<td>Cryoglobulinemia</td>
<td>TPE</td>
<td>I</td>
<td>I</td>
</tr>
<tr>
<td>Cutaneous T-cell lymphoma</td>
<td>Cytapheresis</td>
<td>II</td>
<td>I/III</td>
</tr>
<tr>
<td>Drug overdose and poisoning</td>
<td>TPE</td>
<td>II</td>
<td>II</td>
</tr>
<tr>
<td>Eaton-Lambert syndrome</td>
<td>TPE</td>
<td>II</td>
<td>I</td>
</tr>
<tr>
<td>Guillian-Barré syndrome</td>
<td>TPE</td>
<td>I</td>
<td>I</td>
</tr>
<tr>
<td>Hyperparasitemia (malaria)</td>
<td>Red cell exchange</td>
<td>II</td>
<td>NR</td>
</tr>
<tr>
<td>Hyperviscosity</td>
<td>TPE</td>
<td>I</td>
<td>I</td>
</tr>
<tr>
<td>Leukemia with hyperleukcytosis syndrome</td>
<td>Cytoreduction</td>
<td>I</td>
<td>I</td>
</tr>
<tr>
<td>Multiple sclerosis</td>
<td>TPE/cytapheresis</td>
<td>III</td>
<td>III</td>
</tr>
<tr>
<td>Myasthenia gravis</td>
<td>TPE</td>
<td>I</td>
<td>I</td>
</tr>
<tr>
<td>Peripheral blood progenitor cells for hematopoietic reconstruction</td>
<td>Cytapheresis</td>
<td>I</td>
<td>NR</td>
</tr>
<tr>
<td>Posttransfusion purpura</td>
<td>TPE</td>
<td>I</td>
<td>I</td>
</tr>
<tr>
<td>Rasmussen’s encephalitis</td>
<td>TPE</td>
<td>III</td>
<td>NR</td>
</tr>
<tr>
<td>Sickle cell syndromes</td>
<td>Red cell exchange</td>
<td>I</td>
<td>I</td>
</tr>
<tr>
<td>Systematic lupus erythematosus</td>
<td>Red cell exchange</td>
<td>NR</td>
<td>II</td>
</tr>
<tr>
<td>Thrombocytosis, symptomatic</td>
<td>Cytoreduction</td>
<td>I</td>
<td>I</td>
</tr>
</tbody>
</table>

Category I = standard acceptable therapy; Category II = sufficient evidence to suggest efficacy usually as adjunctive therapy; Category III = inconclusive evidence of efficacy or uncertain risk/benefit ratio; Category IV = lack of efficiency in controlled trials; NR = disorder not ranked

**Table 1.1:** Some diseases treated with apheresis – treatment categories in AABB and ASFA guidelines [29, 30]
1.2.3. Technical equipment

The basic idea of apheresis is expedite the sedimentation process of the various particular components (hematocrit) of blood by exposing the suspension of these particles in plasma to high levels acceleration. This acceleration is provided by the centripetal acceleration of a rotating field. Due to the difference of densities between the blood cells and plasma, the body forces developed by centrifugal acceleration is able to overcome the diffusive forces in the suspension, thereby promoting the separation of cellular components from the plasma. Therefore the right instrumentation is needed. Apheresis depends on instrumentation, and many advances in the practice of apheresis have been linked to advances in instrumentation. In the early 1950s Dr. Cohn developed the first blood separator [31-33], the so called Cohn Centrifuge Spectra (Figure 1.1). It is a device in which decalcified blood flows upwards in a separation chamber, which is rotating at about 2000 rpm [34]. The chamber is first filled. Then it is rotated and the separation process occurs. Finally the different parts are filled through different channels into different bags. This is a batch system, which is characterized by a discontinuous draw-separate-return cycle.

Figure 1.1: The Cohn centrifuge Spectra.

In a further development Latham redesigned the bowl and obtained a new simplified bowl of the separator device, the so called Latham bowl (Figure 1.2) [35]. This model showed such good results [36] that it was put on the market and out of it the company
Haemonetics was founded. These batch systems were further developed and as well IBM developed its own blood separator, the NCI-IBM [37]. It was a more sophisticated model with better efficiencies as the previous models [38]. As well it was the first continuous flow separator. That means the blood flow was continuously flowing in and out of the separator as well the separation process was continuously. Further in time the models became more and more sophisticated and efficient, e.g. the whole process included separation as well as washing. The efficiency was improved by changing the geometry and flow rates. Just a small overview of the different systems: Aminco Celltrifuge II [39, 40], Fenwall CS3000 [41], IBM 2997 [42-44], Cobe Spectra [45, 46]. All systems are continuous flow separators and work on the centrifugal principle.

![Figure 1.2: The Latham bowl.](image)

1.3. Computational Fluid Dynamics (CFD)

Computational fluid dynamics (CFD) is a tool used to study fluid flow. More specifically, CFD is a numerical methodology in which the fluid flow governing partial differential equations are approximated through discretization into algebraic equations, and these equations are solved using iterative techniques with the calculating power of a computer. Using CFD, a computational model that represents a system or device that has to be investigated is constructed to form the flow domain. The discretization of the fluid flow governing partial differential equations takes place at distinct locations in the domain; these discrete points constitute the computational
grid. There are mainly two types of grid: structured and unstructured (see Figure 1.3). The structured grid consists of families of grid lines with the property that members of a single family do not cross each other and cross the member of the other family only once. Afterwards the fluid flow physics are applied to this grid, and a software outputs a prediction of the fluid dynamics.

![unstructured grid](image)

![structured grid](image)

**Figure 1.3:** An unstructured grid over a structured grid

CFD is a sophisticated analysis technique. Computational Fluid Dynamics (CFD) has found its way into all branches of engineering and science. Optimization by such techniques can enhance performance, reduce concept-to-prototype time, produce large savings in equipment and energy costs as well as reduce environmental impact. CFD analysis of centrifugal sedimentation can aid the design and operation of cell separators. Therefore CFD is used as a tool to eliminate several physical experimentation cycles of the design process.

The goal of this work is to develop a tool, which helps us understand better the process of separation, especially for the apheresis process, and confirm the physics of the blood separation process. This tool can later on be used to improve the efficiency of apheresis devices.
2. Theoretical Background

2.1. Blood

The average adult has a blood volume of around six to eight percent of its body weight. That’s for an average adult around five liters. Its duty is to transport many substances (oxygen, carbon dioxide, nutrition, vitamins, etc.), the transport of heat (heating cooling), the transmission of signals (hormones), buffering and the protection of the body. Macroscopically viewed, blood is an incompressible viscous liquid on the base of water with a mean density of 1056 kg/m³ and a viscosity of 3.5 cPoise [47, 48]. Microscopically blood is a suspension of blood cells in plasma. The volumetric fraction of the cellular composition of blood, also called hematocrit, is for male 45% and for female 41% [49, 50]. Hematocrit is composed of red blood cells (RBC), also called erythrocytes, white blood cells (WBC), also called leukocytes, and platelets, also called thrombocytes.

Plasma is the liquid part of the blood. It carries the blood cells and proteins. Plasma consists mainly of water, with dissolved proteins and ions that result in plasma viscosity and density values being higher than those of water. It can be modeled as a Newtonian (constant viscosity) and incompressible fluid if the temperature stays constant. The density lies between 1026 kg/m³ and 1035 kg/m³ [51, 52]. The viscosity is a function of the temperature [53] described as

\[ \mu_{\text{plasma}} = \mu_{37} \exp\left[ \eta (37 - T) \right] \]  

where \( \mu_{37} \) is the viscosity of plasma at 37°C, and \( \eta \) is a temperature coefficient. A value of 0.021°C⁻¹ has been taken [54] for the temperature coefficient. The plasma protein concentration is implicit in the \( \mu_{37} \) term, but it has been assumed that all plasma has the same protein concentration and, therefore, only anticoagulant diluting effects receive further consideration. For processes which are happening outside of the body, the temperature is fixed at 29°C. Hence the viscosity can be calculated, due to Equation (2.1). The viscosity of plasma at body temperature in which the particles are flowing (\( \mu_{37} \)) is 1.4 cPoise [50].

The biconcave, disk-shaped mammalian RBC has a very thin membrane that encapsulates a viscous, liquid hemoglobin solution. It has a regular and mainly constant shape and size. Their outer diameter varies between 7.59 \( \mu \)m and 8.5 \( \mu \)m as
the thickness is of 2.5 μm [55, 56]. They are produced in the bone marrow and have a lifetime of around 120 days inside the body [57]. Their main duty is to provide the cells with oxygen and bring the carbon dioxide away back to the lungs. Due to their extremely high elasticity they can move through very small channels, such as the capillaries. Within the blood cells the RBCs comprise the largest part. They are more than 95% of the volume of the hematocrit. As well they have the greatest density of all the blood cells. It varies from 1095 kg/m³ to 1100 kg/m³ [51, 52]. In special flow situations (very slow flow) they clot and form so called rouleaux. This effect changes the properties of the blood.

The term white blood cell, or leukocyte, stands for a class of five morphologically distinct cells which are in the blood and have many functions. They play a key role in the protective mechanisms of the body against diseases, in tissue inflammation, in wound healing, and in other physiological and pathological processes. Among the formed elements of the blood, WBCs constitute the smallest population, with the ratio of one WBC to about 1000 RBCs. Therefore, in many blood rheological considerations WBCs have been neglected. In comparisons to the other blood cells they are the largest. They have mainly a spherical shape with a diameter from 8μm to 16μm [51, 58]. Their density varies between 1050 kg/m³ and 1085 kg/m³ [59, 60].

Among the blood cells, the platelets are the smallest cellular components of blood. These cells aid the clotting process by clinging to the lining of blood vessels. Platelets are made in the bone marrow and survive stored outside of the body for up to five days. They are not making a large volumetric part of the hematocrit, due to their small size, even though their frequency than is forty time larger WBC frequency. They are irregular, disk shaped cells with a diameter which is from 2μm to 5μm [61]. Their density is the lowest, as it is very similar to the plasma density. It is lower than 1040 kg/m³ [51, 62].

In Table 2.1 the main properties of all three blood cell types are listed.

<table>
<thead>
<tr>
<th></th>
<th>RBC</th>
<th>WBC</th>
<th>Platelets</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shape</td>
<td>Biconcave</td>
<td>spherical</td>
<td>irregular disk</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>1095 - 1100</td>
<td>1050-1085</td>
<td>&gt; 1040</td>
</tr>
<tr>
<td>Surface (μm²)</td>
<td>140</td>
<td>330</td>
<td>28</td>
</tr>
<tr>
<td>Radius (μm)</td>
<td>4</td>
<td>4 - 8</td>
<td>1.5</td>
</tr>
<tr>
<td>Volume (μm³)</td>
<td>92</td>
<td>200</td>
<td>14</td>
</tr>
</tbody>
</table>
Table 2.1: Properties of the blood cells

The density of blood is dependent on the hematocrit. A high hematocrit implies a high density, because all the blood particles are denser than plasma. Therefore, Hawksley [63, 64] developed a relationship between hematocrit and blood density, as described

\[ \rho_{\text{blood}} = \rho_{\text{plasma}} (1 - H) + H \rho_{\text{RBC}} \]  \hspace{1cm} (2.2)

where \( \rho_{\text{blood}} \) is the local density of blood, \( \rho_{\text{plasma}} \) the density of plasma at ambient temperature, \( \rho_{\text{RBC}} \) the density of the RBC and \( H \) the hematocrit. Within Equation (2.2) the hematocrit is based only on the volumetric part of the RBCs. Thus it has been extended [65] incorporating WBCs and platelets and extended to

\[ \rho_{\text{blood}} = \rho_{\text{plasma}} (1 - H) + H_{\text{RBC}} \rho_{\text{RBC}} + H_{\text{WBC}} \rho_{\text{WBC}} + H_{\text{Platelet}} \rho_{\text{Platelet}} \]  \hspace{1cm} (2.3)

\[ H = H_{\text{RBC}} + H_{\text{WBC}} + H_{\text{Platelet}} \]  \hspace{1cm} (2.4)

\( \rho_{\text{WBC}} \) and \( \rho_{\text{Platelet}} \) are the densities of the WBC respectively of the platelets. The hematocrit \( H \) has been split in the volumetric fractions \( H_{\text{RBC}}, H_{\text{WBC}} \) and \( H_{\text{Platelet}} \) of the single cell parts of the hematocrit. The blood density can be calculated through the volumetric fraction of the blood cells.

Similar to the density, blood viscosity is not constant. It is dependent on the hematocrit as well the shear rate. Therefore, various models have been developed to describe bloods viscosity. These models are accurately described in Chapter 5, where the non-Newtonian (shear dependent) behavior of blood is modeled.

2.2. Fluid mechanics

Fluid flow is caused by the action of externally applied forces. Common driving forces include pressure differences, gravity, shear, rotation, and surface tension. They can be classified as surface forces (e.g. shear force, pressure) and body forces (e.g. gravity and inertial forces induced by rotation). While all fluids behave similarly under action of forces, their macroscopic properties differ considerably. These properties must be known if one is to study fluid motion; the most important are density and viscosity. Once all properties are known the problem has to be sufficiently defined and solved. Therefore two different approaches can be used: the Eulerian approach and the Lagrangian approach.
2.2.1. Eulerian approach

Within the Eulerian approach the framework of the fluid stays constant, as it is for an external observer who looks on the fluid. Within the framework the independent variables are the spatial coordinates x, y, z and time t. In order to derive the basic conservation equations in this framework, attention is focused on the fluid which passes through a control volume that is fixed in space. The fluid inside the control volume at any instant in time will consist of different fluid particles from that which was there on the previous instant in time. In the Eulerian approach the principles of conservation of mass, momentum, and energy are applied on the fluid passing through the control volume.

Thus the mass conservation for a fixed control volume is described as

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \]  

with \( \rho \) as the density within the control volume and the velocity vector of the fluid. It shows that the change of mass is equal to the flow of mass in and out of the control volume. Similar to the mass conservation most of the governing equations can be expressed in the form of generalized transport equation on a specific control volume

\[ \frac{\partial \rho \Phi}{\partial t} + \nabla \cdot (\rho \vec{v} \Phi) = \nabla \cdot (\Gamma \nabla \Phi) + S_\Phi \]  

This equation is also known as the generic conservation equation for a quantity \( \Phi \). The first term is describing the transient behavior, the second the convection, the third is the diffusion term and the forth is the source term.

The principle of conservation of momentum is an application of Newton’s second law of motion on a control volume of the fluid. Including all forces acting on the volume and adding to them other external forces it can be rewritten for a fluid control volume as

\[ \rho \frac{\partial u_j}{\partial t} + u_i \frac{\partial \rho}{\partial t} + u_j \frac{\partial}{\partial x_k} (\rho u_k) + \rho u_k \frac{\partial u_j}{\partial x_k} = \frac{\partial \sigma_{ij}}{\partial x_i} + \rho f_j \]  

where \( u \) represents the velocity, the indexes \( k, j, \) and \( i \) are showing the direction, \( \sigma_{ij} \) is the surface tension normal to the area of \( i \) and \( j \), \( u \) is the velocity and \( f \) are additional external forces [66].
The flow problem is finally defined by the boundary and initial conditions. Solving these equations and considering the boundary and initial conditions, the flow can be calculated.

2.2.2. Lagrangian approach

In the Lagrangian approach, attention is fixed on a particular mass of fluid or particle as it flows. Thus the framework will follow the mass of fluid or particle as it flows and change the properties of it, but always the same particle is considered. The principles of mass, momentum, and energy conservation are then applied to this particular element of fluid as it flows, resulting in a set of conservation equations in Lagrangian coordinates. In this reference frame $x, y, z$ and $t$ are no longer independent variables, since if it is known that the particle passed through the coordinates $x_0, y_0, z_0$ and $t_0$, then its position at some later time may be calculated if the velocity components $u, v, w$ are known.

To explain better the Lagrangian approach and to have a better relation to the case to calculate the flow of particles in blood, let’s focus the problem on one blood particle. The coordinate system is always moving on the particle and the framework is the particle itself. The particle is modeled as a stiff and impermeable sphere. Hence there is no flux into or out of the particle as there is no mass generation. As well the particle density is constant. Thus the mass conservation is given as

$$\frac{dp}{dt} + \frac{d(\rho u)}{dx} + \frac{d(\rho v)}{dy} + \frac{d(\rho w)}{dz} = 0$$

is solved. The mass flow in the particle is equal zero and the density is constant.

The momentum conservation equation is defined by applying Newton’s second law of motion on a particle.

$$\frac{d(m\vec{v})}{dt} = \sum \vec{F}_{ext}$$

The change of momentum is equal to the sum of all the external forces acting on the particle. This formulation can then be extended by considering all different forces acting on a spherical particle [67].

The drag force acts upon a particle which is in contact with a fluid or gas. The surrounding fluid is generating a shear stress on the particles surface and so accelerating or decelerating the particle. The drag force $F_{drag}$ is defined as
The drag force is proportional to a drag factor \( c_d \), which is a function of flow conditions and particle shape, the particle surface \( S \), the fluid density, and the square of the velocity difference between particle and the fluid around it.

For a particle spinning about an axis perpendicular to its direction of travel, the speed of the particle, relative to the surrounding fluid, is different on opposite sides of the particle. This results in a larger drag force acting on the lower surface of the particle than on the upper surface. If the drag force is imagined as exerting a sort of pressure on the particle then it can be readily appreciated that unequal drag forces are acting on the particle’s sides, and generating a resultant force towards the side, where the surrounding fluid is moving slower. This force is known as the Magnus force [68-70].

The Magnus force for a spherical particle [71-73] the radius \( r \), the velocity \( v \) and the angular velocity \( \omega \), can be written

\[
F_{\text{Magnus}} = \left[1 + O(Re)\right] \pi r^3 m_{\text{particle}} \rho_{\text{fluid}} \sigma \times \vec{v}
\]  

As in Equation (2.11) can be seen, the drag force is as well dependent on the fluid density, the Reynolds number and the particle mass.

Boussinesq [74, 75] and Basset [76, 77] independently derived an expression for the transient hydrodynamic force (the prevalent name at the time was ‘fluid resistance’) exerted by a quiescent fluid on a rigid particle which has been extended by Oseen [78, 79]. The fluid resistance is composed of the pseudo-steady drag and the ‘history integral term’ or so called Basset force. The Basset force originates from the diffusion of velocity gradients in the infinite fluid and has the effect of an augmented drag. On a particle moving in a fluid Basset history term

\[
F_{\text{Basset}} = 6r^2 \sqrt{\pi \rho_{\text{fluid}} \mu_{\text{fluid}}} \int_0^1 \frac{d\tau}{\sqrt{1 - \tau}} d\tau
\]

The Basset force a function of the particle radius \( r \), the fluid density \( \rho \), and the dynamic fluid viscosity \( \mu \).

Small particles in a shear field experience a lift force perpendicular to the direction of flow. The shear lift originates from the inertia effects in the viscous flow around the particle and is fundamentally different from the aerodynamic lift force. The expression for the inertial shear lift was first obtained by Saffman [80, 81]. That is for a particle with the radius \( r \)
Here is $v$ the kinematic viscosity of the suspending fluid, $\mu_{\text{fluid}}$ the dynamic viscosity of the fluid and $\dot{\gamma}$ is the shear rate of the fluid.

Due to concentration differences there is a particle flow from high concentrated particle zones towards to zones with lower concentrations. The equation describing diffusion is called Ficks law

$$\bar{j} = -D \text{grad} \rho_N$$  \hspace{1cm} (2.14)

The diffusion is mainly described by the diffusion coefficient $D$ and the gradient of the particle concentration $\rho_N$. These give the particle stream (mass flux) vector $\bar{j}$.

The pressure created in the flow field is as well acting on the particle’s surface. If there is a gradient of the pressure, the force due the pressure on the particle’s surface is no longer balanced. Due to the pressure gradient the particles feels a force. This force is

$$F_{\text{dp}} = \iiint p \, dS$$  \hspace{1cm} (2.15)

By integrating the pressure $p$ over the whole particle surface $S$ the resultant force can be calculated.

A particle located in a rotating frame of reference is subject to a centrifugal force. The particle, by its inertia, tends to move in a straight path, away from the rotational center, but the centrifugal force accelerates the particle to the rotational center. This force for the rotational velocity $\omega$ is defined as

$$F_{\text{centr}} = \omega^2 \cdot d \cdot \text{Vol}_{\text{cell}} \cdot (\rho_{\text{fluid}} - \rho_{\text{cell}})$$  \hspace{1cm} (2.16)

where $d$ is the distance of the particle to the rotational axes. It is as well dependent on the particle volume and of the density difference between particle and fluid density.

Due to the rotational nature of the frame, a particle that is moving away normal to the rotational axis must undergo an additional acceleration to compensate the change in linear velocity; this accelerations is provided by the Coriolis force. The Coriolis force is a fictitious force exerted on a body when it moves in a rotating reference frame. It is called a fictitious force because it is a by-product of measuring coordinates with respect to a rotating coordinate system as opposed to an actual "push or pull." It is defined for a particle moving with the velocity $v$ in a rotational field with the speed $\omega$. 

$$F_{\text{cor}} = \omega \times (v - \omega \times r)$$

where $r$ is the position vector of the particle.
\[ F_{\text{Coriolis}} = -2m_{\text{part}} \hat{\omega} \times \hat{v}_{\text{part}} \] (2.17)

with, \( m_{\text{part}} \) as the particle mass and \( \hat{v}_{\text{part}} \) as the velocity of the particle.

2.3. Numerical background

Within this work a hybrid (Eulerian - Lagrangian) method has been used, the so-called particle in cell method. The main idea is to trace the motion of a set of material points (particles), which carry information of the state variables in a Lagrangian way, while the spatial discretization of the suspending fluid is made in an Eulerian frame [82-87].

2.3.1. Flow field calculation

The mass and momentum conservation equations are calculated via a commercially available finite volume solver (CFD-ACE+ of ESI CFD, Huntsville, AL, U.S.A.). The solution domain is divided into a number of cells known as control volumes, called grid elements. In the finite volume approach the governing equations are numerically integrated over each of these computational cells respectively control volumes.

For the integration of the conservation equations two different methods have been used. In the first-order upwind scheme, \( \phi_e \) is taken to be the value of \( \phi \) at the upstream grid point, i.e. equals either \( \phi_c \) or \( \phi_p \) depending on the flow direction at cell face \( e \).

Mathematically, \( \phi \) at this phase can be expressed as

\[
\phi_e^{\text{UP}} = \begin{cases} 
\phi_h & \text{if } v_e^* > 0 \\
\phi_l & \text{if } v_e^* < 0 
\end{cases}
\] (2.18)

As its name implies, this scheme has first-order accuracy and is one of the most stable schemes [88].

The second integration scheme used is the central difference scheme. In the conventional second order accurate central difference scheme, \( \phi_e \) is evaluated by arithmetically averaging the values at cell centers \( P \) and \( E \), assuming that \( \phi \) varies linearly between the two centers, namely,

\[
\phi_e^{\text{CD}} = \Psi_e \phi_P + (1 - \Psi_e) \phi_E
\] (2.19)

where \( \Psi_e \) is the geometrical weighting function at the face \( e \).

An algebraic multigrid technique is used for convergence acceleration. The basic idea of the multigrid solution is to use a hierarchy of grids, from fine to coarse to solve a
set of equations, with each grid being particularly effective for removing errors of wavelength characteristic of the mesh spacing on that grid [89]. Solutions of the three momentum equations yield the three Cartesian components of velocity. Even though pressure is an important flow variable, no governing partial differential equation for pressure is presented. Pressure-based methods utilize the continuity equation to formulate an equation for pressure. Therefore a SIMPLEC scheme [90-92] is used for the pressure-velocity coupling is used.

2.3.2. Particle integration

Knowing the flow field of the surrounding fluid and the properties of the fluid, the forces acting on the particle can be defined. To calculate the particle path, the momentum Equation (2.9) has to be solved. The ordinary differential equations of particle motion are solved using an implicit Euler scheme to alleviate stiffness constraints:

$$\Phi^{n+1} = \Phi^n + f(t_{n+1}, \Phi^{n+1}) \Delta t \tag{2.20}$$

It calculates the value of the variable $\Phi$ at the time step $n+1$, using the values of itself at the previous time step and an integration function. The implicit Euler method produces very smooth solutions and behaves well, even for non-linear equations [88]. Combining Equations (2.9) and (2.20) the new velocities in x and y direction can be calculated at the new time. The new position of the particles is calculated by integrating the velocity. If this calculation step is repeated for various time steps, the path of the particle is given.

The properties and velocity of the fluid is obtained only at the center of the computational cell, but the particles are moving within the whole device, not only at certain points. Thus the velocity of the surrounding fluid has been interpolated at the position where the particle is located. An inverse distance interpolation operator has been used. Thus the specific local fluid property and velocity can be calculated at every point in the domain with

$$v_{\text{point}} = \frac{\sum \left( \frac{1}{d_j} \right)^p \Phi_j}{\sum \left( \frac{1}{d_j} \right)^p} \tag{2.21}$$
with $p = 2$. The property or velocity $\varphi_{\text{point}}$ of the flow at the point where the blood particle is, is a function of the velocity $v_j$ of the cells surrounding the particle (indexed with $j$) and the distance $d_j$ to the cell center of the surrounding computational cells.
3. Simulation of a new generation of sedimentation tank

3.1. Introduction

3.1.1. Scope
Within this work a study in collaboration with Biofluid Systems in Nyon has been made to check shape and functionality of a generation of sedimentation basins. The idea is to develop a small sedimentation basin for the glass industry, where particles with a minimal size of 3 micron can sediment. The sedimentation basin should be smaller, cheaper than existing tanks, and as well, easy to produce.

During the study various simulations are performed, and the efficiency of the new system is calculated. If the simulations show that the sedimentation efficiency of this new geometry is better than the efficiency of existing systems, a prototype is built and tests are performed. The idea is based on having smaller and cheaper sedimentation basins. The first step to be made is to check if this new model is efficient and can compete with already existing models. Using the help of a CFD simulation, a first study can be made without the need and expense of constructing a sedimentation basin. Therefore a first study with CFD avoids the test setting and leads quickly to an ideal solution.

This study is also a step in the development of the model for blood separation. The method used is a first step to the final model of the blood separation program.

3.1.2. Water reserves in the world

Water – the very word brings to mind an image of born recent space voyages – the picture of a blue planet: Earth. Water is the most common mineral on the earth’s surface. It makes up the hydrosphere. The earth and all living on it need fresh water to survive. But how is the situation of the water resources in the world? It is commonly assumed that world’s water supply is huge and infinite. This assumption is false. In fact, of all water on Earth, only 2.5 percent is fresh water, and available fresh water represents less than half of 1 percent of the world’s total water stock.

The total amount of water on the world is estimated around 1.4 billion cubic meters. The largest part is salt water. Only 36 million cubic meters are fresh water, that means usable for human needs [93]. Out of the fresh water amount only 34% is in the water
circulation on the surface. Finally, the renewable water, which is accessible for everybody, is limited to around 35,000 cubic meters [94]. The largest part of fresh water is under ground in sometimes very deep layers. The amount is around 60 times larger, but it isn’t renewed. It does, however, make part of the water cycle. It is accumulated and stored over a long period of time, cannot be restored. When the ground water storages are emptied, they are not refilled and the amount of fresh water is decreased.

The amount of renewable water in the circulation is limited, but the need for water is increasing with the world population. The population is increasing very fast. Within 20 years it should grow by 57 % [95]. With the growing world population the urbanization will also increase. In the next 20 years it will increase by 160% and more people will be living in cities than on countryside [96]. This leads to larger water consumption in cities, for industrial and private purposes. The need of water is not only fundamental for the survival of nature, as well industry needs fresh water for its processes. Water use in industries ranges from hydraulic extraction processes to cleaning, processing cooling and waste disposal, e.g. for the pumping of one barrel petroleum, five barrels of water are needed. Water used by industries is mainly renewable water [95]. Industry is increasing and so are the needs of human. The population is also growing and hence the water consumption is becoming larger. The industry water consumption will double in the next 20 years [96]. Thus, it is not surprising that water related disease is a chief cause of death for children under five years of age [97]. Typical methods of treating available drinking water supplies, from simple to complex technologies are strongly required [98].

Therefore the regeneration of polluted water is imperative. It is an act of self-preservation, because our survival and the survival of all living creatures on earth is dependent on the water. Thus systems are needed which make used and polluted water usable again [99]. Water scarcity problems have been more and more severe around the world and so great attention is being paid to reclamation and reuse of wastewater from municipalities and industrial plants [100].

3.1.3. Wastewater systems

Wastewater systems have been developed since the ancient times of the Roman Empire. They have been developed more and more. Especially with the industrialization it made a number of changes, adapting the system to the current
technologies. Modern wastewater systems are divided into five processes (see Figure 3.1): preliminary treatment (1), primary treatment (2), secondary treatment (3), tertiary treatment (4) and sludge treatment (5) [94, 101, 102].

![Figure 3.1: A modern wastewater system.](image)

The preliminary treatment is the first stage of the water cleaning process. Within it large solid and inorganic material such as paper and plastics are screened. This is followed by the removal of particles such as grit and silt which are abrasive to plant equipment.

Following preliminary treatment, wastewater is passed through a primary sedimentation tank where solid particles of organic material are removed from the suspension by gravity settling. Within this stage the particle size is over 200 μm. The resultant settled primary sludge is raked to the center of the tank where it is concentrated and pumped away for further treatment.

After the primary treatment, the secondary treatment follows. It is a biological process which breaks down dissolved and suspended organic solids by using naturally occurring micro-organisms. It is called the activated sludge process.

The settled wastewater enters aeration tanks where air is blown into the liquid to provide oxygen for mixing and to promote the growth of micro-organisms. The “active biomass” uses the oxygen and consumes organic pollutants and nutrients in the wastewater to grow and reproduce.

From the aeration tanks, the mixture of wastewater and micro-organisms passes into a secondary sedimentation tank (also known as a clarifier) where the biomass settles under gravity to the bottom of the tank and is concentrated as sludge.

The clarified wastewater is discharged from the secondary clarifier and passes through for tertiary treatment.

All wastewater treatment plants use disinfection for tertiary treatment to reduce pathogens, which are micro-organisms which can pose a risk to human health. Chlorine is usually dosed into the treated wastewater stream for disinfection.
Sludge collected during the treatment process contains a large amount of biodegradable material making it amenable to treatment by a different set of microorganisms, called anaerobic bacteria, which do not need oxygen for growth. The gas produced during this anaerobic process contains a large amount of methane. Once the micro-organisms have done their work water is removed from the digested sludge through mechanical means such as centrifuging, or by natural solar evaporation in lagoons. The stable, solid material remaining looks, feels and smells like damp earth and makes ideal conditioner for soil.

3.1.4. Sedimentation basins

As societies developed, reservoirs and storage tanks were constructed. Although constructed for strategic purpose, reservoirs and storage tanks did improve water quality. Various examples are known that predate Christian area. Ancient surface water impounding tanks of Aden were possibly constructed as early as 600 B.C. and rainwater cisterns of ancient Carthage about 150 B.C. [103]. The castellae and piscinae of the Roman aqueduct system performed the function of settling tanks, even though they were not originally intended for that purpose.

The art of sedimentation progressed little until the industrial age and its increased needs of water. Storage reservoirs developed into settling reservoirs. The development of settling basins led to the construction of rectangular masonry settling tanks that assured more even flow distribution and easier sludge removal.

Attempts to make rectangular tanks more cost-effective led to construction of multilayer tanks. Very large diameter (60m) [104] circular tanks also were constructed at an early stage in the development of modern water treatment.

Figure 3.2: A circular sedimentation basin [105].
Other industries, such as wastewater treatment, mineral processing, sugar refinement, and water softening, required forms of sedimentation with specific characteristics. Subsequently, wider applications of successful industrial design were sought [105]. The inclined plate settler also has industrial origins [106], although the theory of inclined settling dates back to the 1920s and '30s [98, 107]. Closely spaced inclined plate systems for wastewater treatment have their origins in Sweden in the 1950s, resulting from the search for high rate treatment processes compact enough to be economically housed against winter weather. Inclined tube systems were spawned in the USA in the '60s.

![Sedimentation basin with lamellas of the '50s](image)

**Figure 3.3:** Sedimentation basin with lamellas of the '50s [106].

The most recent developments have involved combining inclined settling with ballasting a clump of waste particles, also called floc, to reduce plant footprint further [108]. So the models were still further developed but their size did decrease measurably. The smallest sedimentation systems used today have a size has a diameter of 40 meters, with a depth of 5 meters [109-113]. As well there is a variety of systems. All these systems can fully separate particles down to a size of 25 microns.

### 3.1.5. Glass production

Within the production and processing of glass a high amount of water is used for cooling and cleaning. Thus the water is polluted by different materials such as heavy metals and small glass particles [114, 115]. The release of particles in water should be lower than 0.1 kilogram per ton, but today the pollution of the water is 100 times higher, which corresponds to 1% of the weights of the water. The second problem is the size of the particles, which varies between 1 and 60 micrometers. Their size is just at the limit of a sedimenting solid (see Figure 3.4). Due to the relatively high density of glass compared to water, a sedimentation tank has to be used, even if it is suggested
that sedimentation is appropriated only down to particles sizes on the order of 30 microns [116, 117].

The goal of all high rate clarification processes is to reduce the surface area without impairing the stability of the clarification process. As already mentioned the particles are separating from the water due to the density difference and the gravity. To improve the basin efficiency, lamellas are incorporated into the clarificator (see Figure 3.3). The sedimentation area of a lamellar clarificator is higher and so the efficiency of such devices improves.

3.2. Theory

3.2.1. Sedimentation

The particle-fluid separation process of interest is difficult to describe by a theoretical analysis, mainly because the involved particles are not regular in shape, density, or size. Consideration of the theory of ideal systems is, however, a useful guide to interpreting observed behavior in more complex cases.

The general term settling is used to describe all types of particles falling through a liquid under the force of gravity, and settling phenomena in which the particles or aggregates are suspended by hydrodynamic forces only. In order that a particle settles, its density and size has to be large enough. Otherwise the particle would just flow along with the liquid carrying it.

Within the glass production the concentration of particles is of one volumetric percent. Thus within the sedimentation tank settling of particles at low concentration with coalescence or flocculation takes place. As coalescence occurs, particle masses increase and particles settle more rapidly.
When the concentration of particles is small, each particle settles discretely unhindered by the presence of other particles. Starting from the rest, the velocity of a single particle under gravity in a liquid will increase when the density of the particle is greater than the density of the liquid. Acceleration continues until the resistance of the flow through the liquid, or drag, equals the effective weight of the particle. Thereafter, the settling velocity remains essentially constant. This velocity is called the terminal velocity, \( v_t \). The terminal settling velocity depends on various factors related to the particle and liquid.

The general equation for the terminal settling velocity of a single particle is derived by equating the forces on the particle. These forces are the drag force \( f_d \), the buoyancy \( f_b \), and the external gravity \( f_g \).

\[
f_d = f_g - f_b \tag{3.1}
\]

The drag force on a particle traveling in a resistant, quiescent fluid is [118]

\[
f_d = \frac{1}{2} c_D v^2 \rho \frac{A}{d} \tag{3.2}
\]

where  
- \( c_D = \) drag coefficient  
- \( v = \) velocity of particle  
- \( \rho = \) mass density  
- \( A = \) projected area of the particle in the direction of the flow

The difference of gravity force and the buoyancy is a function of the particle volume \( V \), the gravitational constant acceleration \( g \) and the density difference of particle and the surrounding fluid, as described in Equation (3.3)

\[
f_g - f_b = V g (\rho_{\text{particle}} - \rho_{\text{fluid}}) \tag{3.3}
\]

When Equations (3.2) and (3.3) are substituted in Equation 1.1 and the particles are modeled as solid and spherical then the settling velocity can be calculated.

\[
v_t = \left( \frac{4g(\rho_{\text{particle}} - \rho_{\text{fluid}})d}{3c_D \rho_{\text{fluid}}} \right)^{1/2} \tag{3.4}
\]

where \( d \) is the diameter of the sphere. The value of \( v_t \) is the difference in velocity between the particle and the liquid and is essentially independent of the horizontal or vertical movement of the liquid, although in real situations there are secondary forces caused by velocity gradients and so on. Within this project these effects have been neglected based on their minor role.
The Reynolds number is a proportion of the inertia to the viscous force. It describes the nature of the flow as laminar, transitional, or wholly turbulent. For a particle the Reynolds number is defined as

\[ \text{Re}_{\text{Particle}} = \frac{D_{\text{Particle}} \rho_{\text{Fluid}} |v_{\text{Fluid}} - v_{\text{Particle}}|}{\mu_{\text{Fluid}}} \]  

(3.5)

When the Reynolds number of the particle is known the drag coefficient can be calculated. It is a function of the Reynolds number and changes its formulation accordingly. Because of the small velocity difference between the particle and the suspending fluid, as well the small Reynolds number, the flow behavior can be modeled as a Stokes flow where the drag coefficient is

\[ c_d = \frac{24}{\text{Re}} \]  

(3.6)

This substituted in Equation (3.1), gives the terminal velocity for a Stokes flow

\[ v_t = \frac{g (\rho_{\text{particle}} - \rho_{\text{fluid}}) d^2}{18 \mu} \]  

(3.7)

Thus the terminal velocity is a function of the particle size. In Figure 3.5 the settling velocity is graphically depicted for a particle in a moving fluid. After passing the inlet zone, it is carried with constant velocity over the entire sedimentation zone. The settling velocity remains constant over the entire length. Thus the basin has to be long enough, in order that the particle has enough time to settle and does not flow out with the suspending fluid.

![Figure 3.5: Sedimentation of particle which is not flocculating.](image)
Figure 3.6 shows that the sedimentation velocity is increasing with the square of the particle diameter, as described in Equation (3.7). A glass particle with a diameter of 50 μm needs over 15 minutes to settle in a tank with a height of 2 meters and filled with water. If the particle size is doubled, then the sedimentation time is less than 4 minutes. Thus the effect of flocculation improves the sedimentation efficiency much. As the particle size increases, the sedimentation velocity increases proportional to the square.

\[ \frac{d(mv)}{dt} = f_e - f_b - f_d \]  (3.8)

where \( m \) is the particle mass and \( v \) is the velocity of the particle. The mass remains constant, so Equation (3.8) can be integrated and the velocity change can be
calculated. If the vertical velocity of the liquid is higher than the settling velocity, the particle will never settle. The drag force will carry the particle with the fluid.

### 3.2.2. Flocculation

When the concentration of suspended matter is very low, the dispersed particles settle as if they were alone. However, when the concentration of suspended particles is high enough, a particle’s falling speed may increase when it encounters another particle. This is effect is called flocculation.

Particles may join together (coalescence); they then flocculate and settle at an increased velocity, due to the increased particle size. Thus in a tank with a horizontal hydraulic flow the settling trajectory is curved (Figure 3.7). If flocculation is taking place, the particle sedimentation velocity increases during its flow path. If a flocculant agent is present in the fluid the settling velocity increases even more. This is shown in Figure 3.7, where $H$ is the height of the inflow particles, which sediment without the help of flocculation, $v$ is the sedimentation velocity at the specific length. This figure shows so the effect of a flocculation agent, which increases the aggregation process, so that all particles, which enter the tank at the height $H_0$, would settle with the velocity $v_0$. During flocculation particles join together and create a new larger particles. The density of the new particles decreases and accordingly their volume increases [119, 120].

![Figure 3.7: Sedimentation path of flocculating particles, with and without flocculation agent. The particles which are flowing in the basin at height $H$ or lower, will completely settle. With the help of a flocculation agent this height is increased to $H_0$.](image)

29
To model the settling process of the glass particles, flocculation has been included. When two particles encounter each other, they stick together and form a new particle. This new particle has a larger volume than the sum of the volume of the two particles but a smaller density due to porosity. The sedimentation of a flocculating particle is larger than the sedimentation of particles which are not aggregating. Due to flocculation more particles can sediment and the falling height $H$ over a certain length is larger compared to sedimentation without flocculation.

3.2.3. The properties of water
The water molecule may be easily depicted as a simple triangle distinguished by an interatomic angle of 105° owing to the electronegativity of two of its poles. The water molecule has an electric moment that is reflected in its physical and electric properties. Pure water has no color, no taste, no smell, turns to a solid at 0°C and a vapor at 100°C at standard atmospheric pressure. Its density is 997.05 kg·m$^{-3}$ and it is an extremely good solvent. The dynamics viscosity is 1002 Pa·s at a temperature of 25°C. Within the sedimentation tanks, the properties remain mainly constant because of constant temperature and the absence of chemical processes.

3.2.4. The glass particles
The contaminating particles are glass subsidiaries. They are modeled as spheres, in order that the models described before can be used. Glass has properties similar to those of sand. The structure of glass is completely amorphous. It has a density 2400 - 2800 kg/m$^3$ [121].

One volumetric percent of glass particles is within the water, which has been used for the processing of glass. That means within 1 m$^3$ of water is 0.01 m$^3$ of glass. If the particles have a constant diameter of 1 micron, this would correspond to 20 million particles. The data of the particle size and distribution was given by Biofluid Systems (Figure 3.8). Within the contaminated water are glass particles with a diameter between 1 and 60 microns. It can be observed that there is a high concentration of particles with a diameter between 5 and 35 microns. As well 90% of the particles are larger than 3 microns. That means if all particles with a diameter over 3 microns can settle the
water gets a very good quality and reaches the required standards [114, 115]. Thus less than 10% of the waste will remain in the water, and it has only 0.1% of waste in it.

![Figure 3.8: Particle size and distribution in the contaminated water.](image)

3.3. The sedimentation tank geometry

The basic geometry of this new system is given by Biofluid Systems in Nyon. On it the effect of two parameters, blade angle and number of blades, have been investigated.

The idea is based on rectangular sedimentation tanks with blades (see Figure 3.3). Normally there is one inlet of contaminated water and one outlet for the fresh water. The new geometry is smaller. It has one big inlet and many outlets which are
distributed under every blade. In every blade are embedded 5 outlets with the same dimension. Thus the surface of the outflow is larger, the velocity lower and the resident time of the particle increased.

![Figure 3.9: Two dimensional geometry of the basin with data in meter.](image)

The entire tank has a length of 12 meters, a depth of 4 meters and a width of 2 meters, as depicted in Figure 3.9. It is mainly divided in three parts: the inlet, the lower sedimentation chamber and the blades. The inlet is rectangular shaped and has width and height of 2 meters. The lower sedimentation chamber is 10 meters long. At the entrance it has a height of 2 meters, but it decreases linearly until the height is equal zero at the end of the tank. This shape was taken to avoid recirculation zones in a rectangular tank what would lead to dead water zones, where the water is not leaving the sedimentation tank.

The main innovation is that the outlets are integrated and equally distributed in the blades. The blades have a thickness of 5 cm and are hollow. This allows the clean water to leave the tank within the blades (see Figure 3.10). The height of the blade parts is constant 2 meters and the blades are equally distributed on the whole length of the sedimentation tank. Every blade has five outlets.

Within this main geometry 3 different models were tested. For the most general case, the blades have an inclination angle of 60 degrees and the whole system has 10 blades (called case 1). Two parameters of the geometry were checked: the blade angle and the number of blades. To check the effect of the blade angle, the inclination angle was decreased to 45° and the number of blades was still ten (case 2). Case 1 has been extended to a geometry with 50 blades at an inclination angle of 60° (case 3). Out of these three models simulations are made for different particle size and the efficiencies
can be compared and so the main parameter defined. As well the efficiency of the systems is compared with real systems which are much larger.

Figure 3.10: A schematic overview of the blades of the basin with the outflow.
3.4. Methods

3.4.1. The geometries and grids

The sedimentation tank has been modeled as a two-dimensional geometry for all three cases. For each case two different unstructured grids are created with the commercial software Gambit (Fluent Inc., Darmstadt, Hessen, Germany), to run grid independence studies. The grid properties and outlet velocity for the different simulations are listed in Table 3.1.

<table>
<thead>
<tr>
<th></th>
<th>case 1</th>
<th>case 2</th>
<th>case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>blade angle</td>
<td>60°</td>
<td>45°</td>
<td>60°</td>
</tr>
<tr>
<td>number of blades</td>
<td>10</td>
<td>10</td>
<td>50</td>
</tr>
<tr>
<td>grid elements coarse grid</td>
<td>188 979</td>
<td>196 658</td>
<td>294 538</td>
</tr>
<tr>
<td>grid elements fine grid</td>
<td>274 290</td>
<td>279 630</td>
<td>417 153</td>
</tr>
<tr>
<td>outlet velocity (m/s)</td>
<td>0.0241</td>
<td>0.0197</td>
<td>0.00482</td>
</tr>
</tbody>
</table>

**Table 3.1: Grid properties and outflow velocities for the three cases**

3.4.2. The computational scheme

The calculation scheme is an uncoupled mixed Lagrangian Eulerian approach. First the flow field in the sedimentation tank is calculated neglecting the effect of the particles in it. The effect of the particles can be neglected due to the low concentration and due to their small size. Once the flow field is calculated, the particle tracking subroutine is calculating the particle path. It is solving the momentum equation (Equation (3.8)) for every particle at every time step. Therefore, the information of the flow field is obtained. Integrating the momentum equation for every particle, the new particle velocity, and respectively, particle position is calculated. For the time integration, an implicit Euler scheme has been used.

Once the particles have reached the new positions, the subroutine checks the distance between the particles. If there are some which are touching each other, it creates a new one instead of the two previous. Thus flocculation can be simulated.
3.4.3. Simulation conditions

To know the properties of the flow the Reynolds number has to be defined. For this case there are two different Reynolds numbers, one for the particle, as defined in Equation (3.5) and one for the general flow field, as described in Equation (3.9)

\[ Re = \frac{D \rho_{\text{Fluid}} v_{\text{Fluid}}}{\mu_{\text{Fluid}}} \]  

(3.9)

where D is the hydraulic diameter at the entrance, \( v \) the velocity of the fluid at the entrance and \( \rho \) and \( \mu \), density and viscosity of the fluid. The Reynolds number varies for the three cases from 1700 to 7000. Due to this high Reynolds number the flow is turbulent.

Due to the small concentration (one volumetric percent) of particles viscosity and density of the fluid are not affected by their presence. Thus the properties of water will stay constant during the simulation. The density is constant in the entire domain at 1000 kg/m\(^3\), as viscosity is 0.001 Pa s. As well the temperature is constant within the whole basin, it is set at ambient temperature 25°C.

The simulations ran with an upwind scheme using an Algebraic Multigrid Solver (AMG). When the residual of pressure, velocity and of the turbulence criteria reaches a value under \( 10^{-9} \), then the simulation has converged.

3.4.4. Initial conditions

For all simulations, the initial velocity in x - and y- direction was set at one-fifth of the outlet velocity. The initial pressure was set at zero Pascal. These initial conditions helped the simulation to converge quickly.

3.4.5. Boundary conditions

Designers limit the surface water load to 3 m3 m\(^{-2}\) h\(^{-1}\) in classic sedimentation basins [122]. In the smallest existing sedimentation basins this is equivalent to a mass flow of 2000 m\(^3\)/h. To have similar inflow rate the inlet mass flow has been fixed as well been set at 2000 m\(^3\)/h, what corresponds to an inlet velocity of 0.139 m/s.

As required, the mass flow is the same for every outlet in a geometry. This can be done by placing pumps, which are regulating the flow at the outlets. For mass conservation reasons the total mass outflow is equivalent to the mass inflow. Knowing the number of blades (#blades), the blades angle \( \varphi \) and the number of outlet per blades
(constant at five) the velocity at the outlet \( v_{out} \) is known. So on the outflow velocity normal to the blade is calculated as

\[
v_{ex} = \frac{v_{in} \cdot h_{in}}{\# \text{blades} \cdot 0.5 \cdot \frac{h_{sep\_area}}{\sin \varphi}}
\]

(3.10)

where \( v_{in} \) is the inlet velocity, \( h_{in} \) the inlet height and \( h_{sep\_area} \) the height of the part with the blades.

At the walls a no slip condition is set. That means that the velocity at the walls is equal zero.

3.4.6. Particle tracking

Once the calculation of the flow field has converged to a solution, the path of the particles is calculated using a Lagrangian method (Chapter 2.2.2.). There is no effect of the particle flow on the fluid. Thus the flow field of the water will not change. The velocity at a given time \( t \) can be calculated by combining Equations (3.2), (3.3), and (3.8) in Equation (2.20) for every particle. When the new velocity is calculated, it is integrated and the new particle position at given time is calculated. Once all particles are moved to the new position, the subroutine checks the distance between them. If between two particles the distance is lower as the sum their radius, they will become one particle. This new particle has the density as the previous (2500 kg/m\(^3\)) but a new volume. The volume corresponds to the sum of the volume of the single particle.

When all particles are checked, the subroutine calculates the values for the next time step. This procedure is repeated, till all particles which remain in the basin are settled.

The simulation ran for all three models for four different particle diameters: 200, 100, 50 and 25 microns. The reason was to see how the settling behavior changes with the particle size. As well in the given data the particles have diameter form 1 to 60 microns and it could be checked which part of the particles would settle and which will still remain in the water.

At the beginning of the simulations the particles are equally distributed on one line next to the inlet. This assumption has been made because of the low particle concentration, which is one volumetric percent. Thus the simulations had different numbers of particles dependent on their size (Table 3.2).
Table 3.2: Number of particles over their size

<table>
<thead>
<tr>
<th>Diameter (µm)</th>
<th>200</th>
<th>100</th>
<th>50</th>
<th>25</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. particle</td>
<td>1082</td>
<td>2164</td>
<td>4329</td>
<td>8660</td>
</tr>
</tbody>
</table>

The integration time step is set at 0.5 seconds, thus the particles move fast enough within the basin. This time step gives accurate results and the simulations run stable, without neglecting flocculation effects.

### 3.5. Results

As shown in Figure 3.11, Figure 3.12 and Figure 3.13 the shape of the velocity distribution in the horizontal direction is similar for all three cases. At the inlet the velocity is uniform. It decreases between the blades and has even negative values, due to the flow to the outlets. At the beginning of the inclination at the bottom is region of high velocity. That’s due to the high flow rate and decreasing cross section of the basin. After this region the velocity is decreasing towards the last blade. The highest velocity within the basin is 0.15 m/s. Between the blades the horizontal velocity is very low.

![Figure 3.11: Velocity distribution in x direction for Case 1](image)

The high velocity zone at the bottom of the basin is smaller for the Case 2 as for Case 1. A similar effect is shown for the decreasing velocity. Within Case 2 the horizontal velocity decreases faster towards the last blade. This is due to the lower
outflow velocity. Therefore as well the back flow velocity between the blades is lower in Case 2 as in Case 1. The lower inclination angle helps the water flow out.

![Figure 3.12: Velocity distribution in x direction for Case 2.](image)

The horizontal velocity distribution in Case 3 is very smooth (see Figure 3.13). Comparing with the previous cases, the high velocity zone is much smaller. Between the blades the flow is very low in horizontal direction, due to the low outflow velocity. Thus the velocity distribution is smoother and more regular than for Case 1 and 2.

![Figure 3.13: Velocity distribution in x direction for the case3.](image)
Figures 3.14, 3.15, and 3.16 show the vertical velocity distribution. The shape of the velocity looks similar in all three cases, but many differences are shown on the second case. The vertical velocity distribution is characterized by a zero value at the inlet. Its value increases at the bottom of the basin, when its inclination starts. When the fluid is entering the space between the blades it is accelerated in vertical direction. This is the region with the highest vertical velocity. When the fluid is between the blades, its vertical velocity decreases. For the case 1 the values is as well lower than zero.

For Case 1 the vertical velocity varies between -0.0226 m/s and 0.072 m/s. The highest and lowest velocities are located between the blades (see Figure 3.14). The fluid is deviated, thus accelerated, to get between the blades. Thus at the entrance in this region the vertical velocity is the highest over the entire basin. Once the water is between the blades it is moving more slowly in the vertical direction, and it has to flow to the outlets. To reach the two lower outlets, it has to flow back. Hence the vertical velocity takes on negative values.

![Figure 3.14: Velocity distribution in y direction for Case 1.](image)

Comparing the shape of the distribution of Case 1 and Case 2 it can be seen that they are similar, but there are two main differences. Due to the lower outlet velocity, the highest velocity is smaller in Case 2. It is around 0.05 m/s. This is as well an effect of the lower inclination angle of the blades. It is better adapted to the flow and requires a smaller effort for the fluid to change its direction. The flow field in Case 2 has no negative vertical velocities. Thus there is no backflow, to the outlets as in Case 1. Due
to the lower inclination angle and the lower outflow velocity, the water can reach the outlets easier. The lower inclination angle allows a better distribution of the water to the outlets. Thus no backflow is occurs.

![Figure 3.15: Velocity distribution in y direction for Case 2](image)

**Figure 3.15**: Velocity distribution in y direction for Case 2

![Figure 3.16: Velocity distribution in y direction for Case 3.](image)

**Figure 3.16**: Velocity distribution in y direction for Case 3.

Case 3 has the lowest velocities in vertical direction as depicted in Figure 3.16. The maximum velocity in the entire basin is of 0.04 m/s. This velocity is reached in a very small zone where the water is deviated into the region between the blades.
The vertical velocity decreases approaching the top of the basin. Because of the high number of blades, the outflow velocity is much smaller. As well the fluid can be better distributed than in Case 1 and Case 3. The flow resistance is smaller. Consequently lower forces are opposed to the fluid and the velocity changes with less effort.

Figure 3.17 shows the flow streamlines for the Case 1. They are very regular and don’t show any recirculation zone within the device. In the lower part, where no blades are, the flow is mainly parallel with the bottom. Between the blades the fluid is moving towards the outlets. As the mass flow has to be the same for every outlet, the water is flowing downwards. This effect is already shown in Figure 3.14 where the vertical velocity is depicted. The amount of space between the blades the high outflow velocity develop the backflow effect.

![Figure 3.17: Streamlines of the water flow for Case 1.](image)

Comparing the streamlines of the Case 1 and 2 (respectively Figures 3.17 and 3.18) it can be observed that in the lower part the field is similar in both cases. Due to the lower inclination angle of Case 2, no downstream is developing. The flow reaches the outlets in a more direct way. The lower outflow velocity calms the flow. Consequently the water has more time to reach the outlets and is adapting itself easier to the flow field. Having a lower inclination angle supports the equal distribution of the water, thus it adapts better to the outflow boundary condition. The regular flow even prevents the development of vertices, as it does for Case 1.
Within the basin of Case 3 the streamlines are very smooth, as depicted in Figure 3.19. The fluid is flowing directly from the inlet to outlets without any detours. There is no downstream flow between the blades due to the low outlet velocity and the low distance between the blades. The slow moving fluid is opposed by a lower flow resistance, and can change direction more easily. The low velocity gives the fluid more time to change direction, generating a more regular flow pattern. Comparing the streamlines of Case 3 with Case 1, no backflow between is developing. The water flows directly to the outlets. At the end of the basin a recirculation zone is developed. Within this zone the velocity of the flow very low. The main portion of fluid is already distributed in all the previous outlets. This recirculation zone resembles a dead
area of the fluid, because the water is trapped within the vortex. Recirculation zones should be avoided. This zones cannot be used and increase the size of the basin. The main idea of the basin is, that all water which enters, as well leaves the basin.

Figures 3.20 to 3.22 show the streamlines between the first blades. Thus the flow behavior next to the outlets is better represented. As for Case 1 there is a downstream flow at almost every outlet. This is due to the high outlet velocity, steep blade angle and the forced equal mass outflow at every outlet. The shape of the streamlines looks very similar between all blades. Within Case 2 (see Figure 3.21) the less steep blade angle allows the fluid to reach the outlets much easier, so there is no downstream flow. The equal mass outflow causes that fluid is pushed towards higher located outlets. In Case 3 (see Figure 3.22) no backflow appears. The low velocity supports the outflow boundary condition. The flow does not need to be artificially equally distributed at all outlets; it doings this by itself. Thus the streamlines show a direct way to the outlets without any deviations.

Figure 3.20: Streamlines between blades for Case 1.
Figure 3.21: Streamlines between blades for Case 2.

Figure 3.22: Streamlines between blades for Case 3.
Figure 3.23 shows the position of the particles at different time steps, for the case 1. The initial particle diameter is 100 microns. At the beginning of the simulation they are next to the inlet on one line. They then move towards the outlets, respectively towards the blades. After 30 seconds they are at the height of the first blade and still flowing with the water, but have not yet settled. Some particles already move towards the first blade. After 60 more seconds the inflow particle line has been split. Some particles have already settled at the bottom of the basin. On the second blade some particles have flocculated and settled on the blades’ surface. After 300 seconds the free flowing particles reach the back of the basin. In the meantime some particles move towards the previous blades. There, they flocculate and settle, or they leave the basin with the water. The particles which were next to the bottom at the beginning of the simulation settle at the bottom. After 35 minutes the particles have settled or left the basin with the water. If particles settled on the blades surface, they first have to flocculate. This is shown in Figure 3.23 by the larger particle size. Settling of particles without flocculation is possible only on the bottom or on the last three blades. The largest part of the particles settles on the bottom of the basin.

To better analyze the behavior of the different cases, the sedimentation efficiency is evaluated. The sedimentation efficiency is the ratio of settled particles over particles flowing in the basin. Due to the low outflow velocity and the smooth flow field, Case
3, as depicted in Figure 3.24, has the highest sedimentation efficiency. Particles with a diameter over 100 microns are completely separated from the water. Hence all particles with a larger diameter will settle within this geometry. With decreasing particle size the efficiency diminish nearly linear. For inflowing particles with a diameter of 25 micron still over 30% settle.

For the Case 2 the sedimentation efficiency is not so high. Particles with a diameter over 200 microns can fully settle. But only 70% of the particles with a diameter of 100 microns settle. If the particles have a diameter smaller than 25 microns, separation does practically not occur. The efficiency is under 6%.

Case 1 has a similar efficiency as Case 2; it is only slightly lower. For an inflow particle size of 100 microns only 60% settles. When the particle has a diameter of 25 microns, the efficiency is at 3%, and all particles leave the basin with the water.

![Efficiency of three different water cleaning stations](image)

**Figure 3.24:** Cleaning efficiency of the three systems.

### 3.6. Discussion and conclusions

The efficiency is mainly dependent of the flow velocity, resident time in the sedimentation basin and the shape of the flow field [123]. This is shown very well in the comparison of the three cases. Case 1 has the worst efficiency of all three. It has the highest outlet velocity. The velocities within the entire domain are much higher than for the other two cases. Hence the resident time in the basin is short and the
particle does not have enough time to settle. The vertical velocity is especially higher in Case 1. At many points the vertical water velocity is larger than the settling velocity. Within this zone the particles cannot settle. The drag force acting against the gravity is too high and the particles flow with the water. The inclination angle of the blades is decreasing the flow velocity somewhat, but it doesn’t improve the system’s efficiency by much. The flow field becomes smoother, but the velocities are still too high to allow small particles to settle. Thus they are mainly moving with the water and leave the basin. Even the shape of the flow field of Case 1 and Case 2 is similar. Consequently the particles will follow a similar path in both cases. Consequently Case 1 and Case 2 have a similar settling behavior.

Case 3 has the best performance. This is mainly due to the low outflow velocity and the high number of blades. The velocities are much smaller than in the other two cases. Thus the resident time in the basin is larger and the particles have more time to settle. Increasing the number blades, the particles have a larger surface to settle. Thus the possibility of a particle reaching the blade surface increases. The distance to the blade surface as well is smaller and the path to settle gets shorter. Consequently it is easier for it to settle. The vertical velocity in Case 3 is much lower. A falling particle encounters less drag resistance and can settle. Thus the combination of larger number of blades and lower flow velocities leads to a much higher efficiency of Case 3 than the other two cases.

Flocculation is very important for settling. As shown in Figure 3.23 the flocculation process helps the particle to sediment. If they would flow as single particle in the water, they would never settle. But by increasing their size, they increase as well their settling velocity and can sediment.

Increasing the number of blades can be related to improving efficiency. There is the only limitation given by the length of the geometry. A number of 50 blades on a length of 10 meters is the upper limit. If more blades should be set over this length the basin would not be technically feasible. Like the number of blades a low blade angle supports the settling of the particles. The limit is reached at an angle of 45°, where the flow field is not disturbed much. For higher angles the performance decreases, because the fluid is opposed to a higher resistance. But comparing the effect of the inclination angle and the number of blades on the basin efficiency, the effect of the blade angle can be neglected (Figure 3.24).
Compared with existing systems these systems have a low efficiency. Within existing systems particle down to 30 microns can fully settle. The existing systems are much larger and have larger inlet cross-section. Thus the resident time is larger and the velocities are much lower. Consequently particles have more time to settle. For the same mass flow the velocity, in existing systems, is much smaller. This helps as well the particle in the sedimentation process. The lower fluid velocity avoids the development of vortices and facilitates the development of a regular flow field. The behavior in these systems can nearly be compared with sedimentation in a standing fluid.

Their only advantage of these new systems is their size. They are cheaper, more compact and take less space than existing systems [111-113]. They can be used as well for small industries. At the same time their size is the main weakness of these new systems. Due to their short length the resident time of the particles is extremely short. Also the inflow velocity is very high on account of the small inlet cross section area. To compete with existing industrial solutions, they should be larger. But if they are larger, the effect of having a compact system is lost. The regulation of the mass outflow makes the handling and production of the basin complicated, thus prohibiting it from being competitive on the market of sedimentation basins.

This chapter is a first step in the development of a subroutine for a commercial CFD solver to simulate the particle separation process. It shows that sedimentation, including flocculation, can be simulated with the same approach. For low particle concentration in a flow, the effect of the particle on the fluid can be neglected. Thus separation process can be investigated and the pertinent parameters of the process can be revealed, without the need for expensive experiments.

Within the work, a stable computational method was programmed to obtain reliable results for the particle tracking methods. First some test simulations ran with an explicit method. This model didn’t lead the simulations to convergence. It was very unstable. Therefore the implicit Euler formulation has been taken to calculate the particle movement. This method gave reliable results and leads to convergence. This is a first fundamental step to get to final solution of the simulation of an apheresis device.

I think that people should do more to save water and be more informed about the scarcity of water that we have. Water is basic for the surviving of human and the whole biological system. Therefore, I think engineering should find solutions to avoid
water pollution and systems which can make water drinkable. If we, as the population, were more sensitized on this problem and we may learn to better appreciate this invaluable resource and take a more active role in its conservation.
4. Simulation of the Blood Separation Process using a Newtonian model

4.1. Introduction

The process of apheresis begins with the removal of whole blood from a patient or donor. Within an instrument that is essentially designed as a centrifuge, the components of whole blood are subjected to intense acceleration by rotation and therefore quickly separated. One of the separated portions is then withdrawn and the remaining components are retransfused into the patient or donor. Blood separation is implemented in therapeutical treatments as well as in storage of blood.

Computer Aided Design and, in particular, Computational Fluid Dynamics (CFD) have found their way into all branches of engineering and science. Optimization by such techniques can enhance performance, reduce concept-to-prototype time, produce large savings in equipment and energy costs as well as reduce environmental impact. CFD analysis of centrifugal sedimentation can aid the design and operation of cell separators. Therefore CFD is used as a tool to eliminate several physical experimentation cycles of the design process.

Within a first step the model of the blood separation process has been developed, where the viscosity remains constant and only the hematocrit changes. The hematocrit has effects on the blood cells and on the flow field. Thus the model is checked on convergence extending the subroutine used in Chapter 3, by changing the local density of the fluid during the simulations. This affects as well a back coupling of the particle flow to flow field calculation.

4.2. The blood separator geometry

A flow-through chamber located in a centrifugal field to effect separation is used for continuous flow centrifugal cell separation. The simulation geometry has been defined so the results can be compared with experimental results of Brown [54]. Brown performed experiments in a circular bowl (Figure 4.1) at a constant mid-slot radius of 7.02 cm, a chamber thickness of 4 mm and two different lengths of 13 cm and 43 cm. Most of the experiments were performed on the shorter bowl. The centrifuge was operated at rotational speeds of from as low as 1,425 rpm to as high as 3,250 rpm with most of the experiments conducted at 3,000 rpm. This corresponds to an acceleration
between 159 to 803 g’s (1 g = 9.80 m/s²), although most of the experiments were conducted at 700 g’s.

**Figure 4.1:** The three dimensional separation bowl of Browns [54] experiments.

For the computational calculation, the chamber has been unfolded and projected on the x-y plane (Figure 4.2). At the left side of the chamber, blood is continuously introduced at an initial hematocrit. The acceleration of the chamber around the rotation axis gives rise to a centrifugal force, which causes the cells to settle towards the outer wall of the chamber. The cells with a density which is higher than the introduced blood fall towards the outer wall. Those nearest to the outer wall pile up and build a packed cell bed. The packed cell bed continues to grow while cells continue to enter it near the flow inlet but compacts once all possible cells have been captured.

**Figure 4.2:** The unfolded two dimensional separator geometry.
The geometry of the chamber has a similar shape as that used by Brown and Sartory [54, 124]. The chamber is composed of three parts (Figure 4.2). At the inlet, which has a width of 1 mm and a length of 2.5 mm, the flow develops from a constant velocity profile to a parabolic profile. The central region is the main part of the separation chamber. It has a length of 13 cm and a width of 4 mm. To avoid the development of recirculation vortices, as it happens in tubes with sudden expansions [125], the separation chamber has a smooth inflow contour. After the expansion, the chamber has a constant width. This is the region in which the separation process takes place. At the end of the center region, the chamber splits into two outlets. This third part is composed of two small tubes in the upper and lower regions. They each have a width of 0.5 mm and length of 2.5 mm.

4.3. The particle model

Blood is often modeled as a suspension of different particles but behaves more like an emulsion for fast flows. The suspending fluid in blood is the plasma. Plasma consists mainly of water with dissolved proteins and ions which increase the viscosity and density values higher than those of water, and can be modeled as a Newtonian, incompressible fluid if the temperature remains constant. Plasmas properties and constituents have already been described in Chapter 2.1.

Within the plasma, the blood particles are moving and a variety of pressure and body forces are acting upon them. Using a Lagrangian approach their path within the flow domain can be determined by summing these forces. This method solves the momentum equation for every single particle, which is modelled as a sphere or as a circle in 2-D, defining all forces acting on it.

\[
\frac{d(m\vec{v})}{dt} = \sum \vec{F}_{\text{ext}}
\]  

That means that the change of momentum is equal to the sum of all the external forces acting on the particle. This formulation can then be extended by considering all different forces acting on a spherical particle [67]. There are several forces acting on the particle: the centrifugal force due the rotational field, the buoyancy force inverse to the centrifugal force, the Coriolis force, the drag force due to the friction with the surrounding fluid and diffusion, the Magnus effect, the pressure gradient and the ‘history integration term’ (so called Basset term). All these terms have been defined in Chapter 2.2.2.
The overriding component of these forces is the balance of centrifugal and buoyancy forces, which implies the separation of the blood cells from the plasma. The balance is governed predominantly by the centrifugal force (Equation (2.16)). The balance between centrifugal and buoyancy force is dependent of the particle density as well of the local density of the surrounding fluid. The local density is defined by the extended formulation of Hawksley (Equations (2.3) and (2.4)).

It is further assumed that the vector cross product $\omega \times V$ remains small compared with the centrifugal acceleration and the Coriolis forces can be ignored [126, 127]. Calculations show that the Coriolis force is 400 times smaller than the centrifugal force.

It must be pointed out that, in the case of a particle present in a fluid, which itself is in motion, there are two relevant Reynolds numbers based on the velocity of the flow and on the relative velocity of the sphere. These two Reynolds numbers are defined as

$$Re_m = \frac{D_{\text{separator}} \rho_{\text{fluid}} V_{\text{fluid}}}{\mu_{\text{fluid}}}$$

$$Re_{\text{particle}} = \frac{D_{\text{particle}} \rho_{\text{fluid}} |V_{\text{fluid}} - u_{\text{particle}}|}{\mu_{\text{fluid}}}$$

It is evident that $Re_m >> Re_{\text{particle}}$. The mean Reynolds number ($Re_m$) in the flow chamber is lower than 10 over the entire flow domain.

The hypothetical and real separation chambers addressed in this work all have lengths that are much larger than their respective thickness (Figure 4.2), and a reduced Reynolds number analysis [128] concludes that viscous forces will dominate over the inertial forces and that the flow will remain laminar. For this reason the particles are moving relatively slowly in the viscous fluid. The Reynolds number for the particles is lower than unity.

The particles are moving within the separator because of the flow field of the surrounding fluid and the forces acting on them. Hence, on every particle moving within the fluid the drag force can be obtained from,

$$F_{\text{drag}} = \frac{1}{2} c_D S_{\text{part}} \rho_{\text{fluid}} (V_{\text{fluid}} - V_{\text{part}}) |V_{\text{fluid}} - V_{\text{part}}|$$

where $c_D$ is the drag coefficient, $S_{\text{part}}$ is the surface of the blood particle, $\rho_{\text{fluid}}$ is the density of the surrounding fluid and in parenthesis is the difference in velocity between the suspending fluid and the particle. The drag coefficient $c_D$ is dependent on the particle Reynolds number. This Reynolds number of the particle is consistently smaller than unity, and therefore the Stokes formula can be used for determining the drag coefficient,
Due to concentration differences there is a particle flow from high concentrated particle zones towards zones with lower concentrations. The equation describing diffusion is called Fick’s law (Equation (2.14)). The diffusion is mainly described by the diffusion coefficient $D$ and the gradient of the particle concentration $\rho_N$. These give the particle stream vector $\vec{j}$. The packed cell bed is roughly 1 to 2 mm thick and has a smooth continuous distribution of hematocrit; cell migration due to diffusion forces has been shown to be negligible for the case of sedimentation due to gravity [129]. It has also been shown that the diffusion force is four orders of magnitude smaller when compared with the effect of drag and centrifugal force. This is valid for the case of Huang et al. [130] where the width of the separator is much smaller than the length of the centrifugal chamber. As approximated by Svedberg and Pederson [131] the diffusion force term is proportional to the chamber width. Thus the diffusivity will be even smaller in the chamber under study, because of the smaller width of the chamber and higher sedimentation forces attributed to the centrifugal acceleration.

A spinning object creates a sort of whirlpool of rotating fluid about itself. On the side where the motion of the whirlpool is in the same direction as that of the fluid stream is exposed, the velocity will be enhanced. On the opposite side where the motions are opposed, the velocity will be decreased. Consequently there is an unbalanced force perpendicular to the stream. This force is called the Magnus force. Comparing the Magnus force with the centrifugal and the drag force, it is a factor over 1000 times smaller then these two forces, and thus neglected [132-134].

The blood particles are modelled as very small rigid circular bodies. A pressure gradient, which is imposed from the inlet and outlet conditions, has an effect on every particle. The size of the particles is very small and the other forces acting on the particle are at least a factor of 100 larger. Thus the effect of the pressure gradient on the particle can be neglected.

Boussinesq [74] and Basset [77] independently derived an expression for the transient hydrodynamic force (the prevalent name at the time was ‘fluid resistance’) exerted by a quiescent fluid on a rigid particle. The fluid resistance is composed of the pseudo-steady-drag and the ‘history integral term’ or so called Basset force. The Basset force

$$c_d = \frac{24}{\text{Re}}$$ (4.4)
originates from the diffusion of velocity gradients in the infinite fluid. Michaelides and Feng [135, 136] as well Vojir and Michaelides [137] showed that the Basset force is relevant when the ratio of the fluid density and particle density is greater than 0.002 and lower than 0.7. Within the flow field this ratio is varies between 0.95 and unity. Thus for the case computed in this work the Basset force can be neglected.

The shear of the fluid itself may induce a lateral force on the particle, even in absence of rotation. This is called the Saffman force (Equation (2.13)). The Saffman force is neglected for fluid flows with low Reynolds numbers [127, 138, 139]. The Saffman force is a factor over 100 smaller than the drag force acting on the particle and is neglected.

Once the total force is calculated, it can be integrated and the velocity change of the particle calculated. If the velocity is known it can be integrated a second time to obtain the change of position of the blood cell. Because of the unsteady nature of the process, the momentum equation is solved at every time step and in this manner the path of a blood cell in the separator is calculated.

The flow field is determined using an Eulerian approach. For the given domain and fluid properties, the flow is obtained by solving the momentum and the mass conservation equations. Apheresis is a transient process; the flow field and fluid properties change until asymptotically reaching a quasi-steady behaviour for a continuous process.

### 4.4. The computational scheme

Within the simulation of the separation process, two different calculation perspectives are used: the Eulerian perspective, where the entire flow field is calculated with respect to a stationary frame of reference, and the Lagrangian perspective, where the particle motion in the fluid is calculated (Figure 4.3) with respect to the frame of reference of the moving particle.

At begin of the simulation all particles are initialized at a position and all initial values of the flow field are given. Once all initial files are created the simulation process starts. The flow field is calculated for half a time step \( \frac{dt}{2} \). When it converges, the flow field is recalculated for a second time at the time \( t+\frac{dt}{2} \) until it converges and the time is increased for half a time step \( \frac{dt}{2} \). This procedure helps the simulation run faster and have more accurate results. When the flow field calculation converges the second time, the momentum equation is solved for each particle. After the integration
the particles are in a new position in the flow field. Due to this new distribution of the particles the local density in the separator is recalculated. Once the new density is calculated for every computational cell, it is set in the geometry and the flow field is recalculated for the new time. This process continues until the flow reaches a quasi steady behavior.

Figure 4.3: The calculation scheme.
4.4.1. Flow field calculation

Most of the governing equations can be expressed in the form of the generalized transport Equation (2.6) for a quantity \( \Phi \), which is moving within the geometry. The continuity Equation (2.5), which governs mass conservation, requires special attention because it cannot be written in the form of the general convection-diffusion equation. Moreover, it is used to determine the pressure field in the pressure-based method as employed in the solver.

The mass and momentum conservation equations for the flow field are calculated via a commercially available multi-physics finite volume solver called CFD-ACE+ of ESI CFD, Huntsville, AL, U.S.A, which is using an Eulerian framework. The platform utilized employs the integral form of the conservation equations as its starting point. The solution domain is subdivided into a finite number of adjacent control volumes, and the conservation equations are applied to each control volume. At the center of each control volume lies a computational node at which the variable values are calculated.

Upwind, central and higher order methods have been tested for the spatial discretization of the governing equations. An algebraic multigrid technique is used for convergence acceleration and a SIMPLEC scheme [90-92] is used for the pressure-velocity coupling.

4.4.2. Particle integration

Once the calculation of the flow field has converged to a solution, the paths of the particles are calculated using a Lagrangian method. The ordinary differential equations of particle motion are solved using an implicit Euler scheme (Equation (2.20)) to alleviate stiffness constraints.

Solving the momentum equation for the new velocity combining Equations (2.16), (4.1) and (4.3), the new velocities in x and y direction can be calculated at the new time. The new position of the particles is calculated by integrating the velocity.

The particles are dispersed in the fluid field and, in general, their positions do not correspond with the points at which the Eulerian field is defined. For this reason the velocity field needs to be interpolated onto the particle position. For the evaluation of the velocity at the particle position, an inverse distance interpolation operator has been used (Equation (2.21)), with the exponent \( p \) equal to two.
4.4.3. Density calculation

Once all particles have been displaced to their new positions, the local values of hematocrit are adjusted (Figure 4.3). Thus in every computational cell the number and type of particles are counted and the density locally calculated. To calculate the density the Equations (2.3) and (2.4) have been discretized and reformulated in Equation (4.5)

\[
\rho_{\text{ComputationalCell}} = \frac{\sum_{i=1}^{\text{tot cell}} \left( \rho_i N_i A_i \right) + \rho_{\text{plasma}} \cdot A_{\text{plasma}}}{A_{\text{ComputationalCell}}}
\]

(4.5)

The density is a volumetric mean value of the number of particles and plasma in the computational cell. Therefore the density and cross-sectional area (for the two dimensional case) of the particles are needed. After the program calculates the new values for the entire grid, it sets the local densities and restarts the calculation loop for the next time step.

4.5. The simulation conditions

4.5.1. The geometry grid

On this geometry, an unstructured triangular grid was constructed with a generator (Gambit, Fluent Inc., Darmstadt, Hessen, Germany). The choice of an unstructured grid has been made due to computational speed reasons. The speed of the computations with an unstructured grid over a structured grid was increased by a factor of four when implementing user written subroutines which interacted with the commercial CFD code. For grid independence studies of the model, two grids of differing refinement were created. The coarse grid was comprised of 50,000 elements and the fine grid had 150,000 grid elements. The refinement of the second grid was chosen so that one computational cell contains space for at least 10 representative particles [140, 141]. Thus the grid with 150,000 elements is the smallest grid for the representative particle size.

4.5.2. Simulation settings

The simulations have been defined for comparison with experimental results of Brown [54]. Brown performed experiments in a circular bowl (see Figure 4.1) at a constant mid-slot radius of 7.02 cm, a chamber thickness of 4 mm and two different lengths of 13 cm and 43 cm. Most of the experiments were performed on the shorter
bowl. The centrifuge was operated at rotational speeds of from as low as 1,425 rpm to as high as 3,250 rpm with most of the experiments conducted at 3,000 rpm. This corresponds to an acceleration between 159 to 803 g’s (1 g = 9.80 m/s²), although most of the experiments were conducted at 700 g’s. The blood flow rate at varied between 15 to 130 ml/min and the inlet hematocrit was adjusted from 0.26 to 0.52. These data were used to set the simulation conditions.

The computational domain rotates about an axis which is at a radial distance of 7.02 cm from the axis of symmetry of the separation device. The rotation speed \( \omega \) is 314 rad/s, which corresponds to 3000 rpm. The viscosity of plasma is fixed at a value of 1.65 cp to obtain results for the preliminary study of the computational method. The density changes during the process and is calculated on the basis of the hematocrit in a computational cell. The time step is set at 0.05 seconds to accurately capture the transient behavior of the process.

Uniformly mixed blood with a hematocrit of 0.3 enters the inlet with a uniform velocity profile of 0.01 m/s. A constant pressure boundary condition is specified at the two outlets. At the walls a no-slip velocity condition is set.

The initial velocity is set in the entire flow domain at 0.005 m/s in the x-direction. At the beginning of the simulation the density is uniformly set at 1050 kg/m³. The flow calculation fully converges when it reaches a residual of \( 10^{-9} \) for the velocities and pressure at each time step.

Each computational particle is not representing one blood cell but a certain number of particles (otherwise, prohibitively high numbers would be necessary). Therefore a representative number has been introduced. This number indicates the number of blood cells one computational particle represents. For this simulation the representative number was arbitrarily set to 10.

The initial and inlet hematocrit were fixed at 30%. Out of these values the initial number of blood particles was calculated. This corresponds to around 350,000 particles at the beginning of the simulation.

The ranges of the parameter values of the blood particles are as indicated in Table 2.1 [19, 142]. The radius of the RBCs is 4 \( \mu \)m, for the WBCs 6 \( \mu \)m, and for the platelets 1.5 \( \mu \)m. The density of a RBC is set at 1100 kg/m³, the density of a WBC at 1070 kg/m³ and the platelets have the density of 1050 kg/m³. The particles experience fully elastic collision with the walls. This is assumed because the time step \( dt \) is small and...
the particle velocities near the wall are generally very small by the no-slip velocity boundary condition.

4.6. Results

4.6.1. Grid independence

The simulation ran on two different grids, a coarse and a fine grid. Figure 4.4 shows the hematocrit at three different cross sections (x=4 cm, 7 cm, 11 cm) for the two different grids.

![Hematocrit profiles at three different cross-sections for the coarse (dashed line) and fine grid (dotted line).](image)

**Figure 4.4:** Hematocrit profiles at three different cross-sections for the coarse (dashed line) and fine grid (dotted line).

The fine grid reaches the limitations set by the size of the blood particles. Grids containing cells physically smaller than blood particles would disturb the simulation results since the simulation procedure was developed with the Lagrangian particle approach. Comparing these two grids, it was shown that the velocity distribution is
nearly identical for both cases. The particle distribution, respectively the concentration of the blood particles, does not change. The maximal difference of the concentration of particles is approximately one percent, while the mean difference of concentration of the two different grids is less than half a percent, thus validating the grid independence of the solutions.

4.6.2. Concentration of blood cells

In Figure 4.5, the concentration of the RBCs, WBCs and platelets is shown over the entire geometry. At the inlet the RBCs and the platelets are mixed homogeneously. Because of the expansion, the RBCs settle near the inlet and build a small, highly concentrated cell bed. In the central region the packed cell bed thickens and the effects of the expansion disappear. The platelets and RBCs are nearly demixed. Next to the end of the geometry, RBCs and platelets are effectively separated. A platelet layer has developed over the RBC layer.

![Figure 4.5: The concentration of the RBCs, WBCs and platelets over the separation geometry [54, 129].](image)

WBCs cannot be completely demixed from the RBCs, as shown in Figure 4.5. Similar to the platelets, the WBCs are separated at the central region between 0.04 m and 0.1 m. Because of their relatively lower density, WBCs move out of the zones where
the concentration of the RBCs is higher than 0.8. This process starts in the zone where the RBCs are already tightly packed. The results can be compared with the experiments [54, 129].

![Hematocrit development during the process over the width of the geometry next to the outlet](image)

**Figure 4.6:** Hematocrit development during the process over the width of the geometry next to the outlet [129].

It is interesting to highlight how the concentration profile changes during the separation process. Figure 4.6 shows the hematocrit over the width of the geometry at \( x = 0.11 \) m. The different lines represent the hematocrit at five different time steps: after 2, 6, 12, 18 and 24 seconds. It can be observed that the hematocrit at the beginning of the process is nearly uniform and increases with time at the bottom of the geometry, while it decreases at the top the geometry. After 18 seconds a quasi steady state is reached and the particles are settled. There is no significant change in the profile form after 24 seconds compared with the profile after 18 seconds. The hematocrit is relatively high at the bottom and reaches nearly zero at the center. It is not equal to zero over the middle of the width due to the bulk motion of the platelets.
outside the packed cell bed, but the platelets are much smaller than the RBCs and are found in a lower frequency, so the hematocrit is relatively low.

4.6.3. Separation efficiency

To compare the results of the simulations with experimental results the separation efficiency $\text{eff}_{\text{separation}}$ is introduced.

$$\text{eff}_{\text{separation}} = 1 - \frac{c_{\text{PCB, out}}}{c_{\text{in}}}$$ (4.6)

The term $c_{\text{PCB, out}}$ is the concentration of a particle type at the outlet of the packed cell bed and $c_{\text{in}}$ is the inflow concentration. Separation efficiency is defined as the elimination of any particular cell type from the packed cell bed at the outlet.

**Figure 4.7:** Platelet separation efficiency plotted against to plasma separation efficiency for the simulation and the experiments. The simulation were performed at an inlet hematocrit of 0.3 and inlet Reynolds number of 10. The data indicate that
platelets are swept out of the packed cell bed by the plasma for simulation and the experiments.

Figure 4.7 shows platelet against plasma separation efficiency and as the graph indicates, the platelet separation efficiency tracks the plasma separation and confirms that platelets are flowing along with the plasma. The efficiency is calculated within the packed cell bed at the outlets. At each outlet at least 10 different heights were identified and the efficiencies at these heights were calculated, averaged over a period of time and then reported in Figure 4.7. The single data points of the experiments are not attributed to any specific settings. They are collected over a period of time and then plotted. The simulation data points were collected at different locations in the packed cell bed at the outlets. As shown in Figure 4.7, the separation efficiencies of platelet and plasma are close to the 45° line. Hence the platelets flow with the plasma. The graph shows that the results of the experiment [54] match well results of the computational simulation. The results are nearly identical for efficiencies greater than 80%. Figure 4.7 can be compared with Figure 4.5, where the results are represented in a different manner. It shows that the platelets are moving out of the packed cell bed of RBC and moving with the separated plasma.

The leukocyte separation efficiency is high at a packed cell concentration over 0.7, as plotted in Figure 4.8. The efficiency is calculated in the packed cell bed at the outlets. The scattered data points are not attributed to specific experimental settings, because the author of the experiments did not attribute the data to any specific settings. The simulation data are taken at different locations and averaged over a host of time periods at the outlets. The data show clusters of points, a small yield at hematocrit in the high 0.7 and the low 0.8, with the remainder of leukocytes emerging at hematocrit in the high 0.8 and the low 0.9. Within Figure 4.8 the comparison of the separation efficiency of the simulation with the experimental data [54] shows a good agreement.
Figure 4.8: WBC separation efficiency is plotted against packed cell bed hematocrit at the outlets for simulation and experiments [54]. The simulation were performed at an inlet hematocrit of 0.3 and inlet Reynolds number of 10. The data point appear to be clustered about low and high yields values.

4.6.4. Particle tracking

The simulation calculates the location of every particle group. As a result, the history of every “representative” particle can be followed. Figure 4.9 shows the particles within the flow domain in the quasi steady state. It shows that the flow path of every single particle can be tracked through time. The platelets are separated quickly from the RBC. Due to their low concentration, it is difficult to find WBCs in this region, but closer inspection reveals their location and separation behavior.
4.7. Discussion and conclusions

This chapter presents a new method to simulate the separation process through CFD. The model was conceptualized, implemented and verified on the basis of published experimental data. It was shown that this model delivers credible results on a simple geometry, giving a practical method to simulate apheresis, which can later on be applied to different separator geometries in the pursuit of performance enhancement.

Comparing the results of the simulations with the experimental data [54, 124], one observes that they match well. The general form of the packed cell bed closely resembles that obtained in the referenced experiments [6]. The separation efficiency is nearly the same in the simulation as in the experiments. The platelets are moving with the plasma and are completely separated from the RBCs. Within the second region of the separator, where the x-length is greater than 4 cm and less than 7 cm, the platelets build a cell layer in the middle region. This layer is nearly completely developed in
the last region of the separation device. This occurs because there is a packed RBC layer at the bottom, which pushes against the platelets. The top contains only plasma and platelets. In this manner, the platelets are pushed toward the bottom, due to the relatively lower density of the platelets to the plasma, which promotes the building of a platelet layer. The platelets are pushed towards the bottom until they reach the packed cell layer of the RBCs. Thus the platelets could build a completely demixed packed cell bed, but due to their relatively small size and low density, this process requires comparably more time. Platelet separation efficiency is solely dependent on plasma separation efficiency. The density of plasma and platelet is very similar and so the platelets flow with the plasma. It is difficult to separate plasma and platelets. Plasma is still left in regions in the packed cell bed where the RBC concentration is not prohibitively high, thus a cluster with lower plasma and platelet efficiency arises. However, plasma and platelets gradually approach complete separation, which is depicted in Figure 4.7 by the development of a cluster in the region defined by high separation efficiencies. Due to the large density difference between plasma, respectively platelet, and RBC they are separated very well and form the high efficiency cluster in Figure 4.7.

The WBC separation efficiency also compares favorably with experiments. The WBCs pass over a hematocrit of 0.8. When the hematocrit is lower than 0.7, the WBCs travel toward the bottom of the packed bed because the necessary reaction force provided by the fluidized bed to accelerate the particle about the rotational axis is greater than the buoyancy force generated by the difference in the density of the WBC and the density of the fluid with hematocrit lower than 0.7. The clustering of the WBCs in Figure 4.8 is due to the distribution of the particles at the inlet, the flow pattern of it and the resistance of the packed cell bed. At the inlet the packed cell bed begins to form and behaves as a porous medium. It has a flow resistance which is high enough to effectively curb the exit of WBCs from the packed cell bed as well as the entrance of WBCs from the free stream. The WBCs in the packed cell bed are moving along the region with a hematocrit of 0.8 where the density corresponds to WBC density; thus they are moving mainly with this region. This characteristic of the effective “filtration” of the WBCs along with the resistance to the entrance and exit of the WBCs in the packed bed explains the development of the two clusters in Figure 4.8. It is presumed that the description of the physical forces in the simulations is sufficient to capture this phenomena of WBC separation based on the comparison
of the results against the experimental data in Figure 4.8. The frequency of the leukocytes is very small compared with that of the erythrocytes, keeping their effect on the entire process to a minimum.

Out of this new computational model, which mimics the apheresis process in a satisfactory manner, the first step of a practical tool has been developed to replace detailed experimental investigation at the first stages of the design cycle. Within the post-processing of the simulation, the most important properties of the geometry and the physical conditions, such as rotational velocity, inlet and outlet conditions can be evaluated for the relevant parameters. After the post-processing, these parameters can be changed and the simulation with optimised conditions can be performed. This can be iterated until the separator efficiency reaches an optimum.

This work produced simulation results that compare well with experimental data, despite working with a two-dimensional geometry to keep the computation power requirement in check. This choice was made because the largest effect on the process comes from the cross-sectional shape of the separator. Height has a small effect on the separation, as well as the gravitational force. The results showed that the relevant forces in the blood separation process are the centrifugal, buoyancy and drag force. All other effects as diffusion, Magnus effect, the Basset term, pressure gradient, the Coriolis force can be safely neglected.
5. Non-Newtonian simulation of the blood separation process

5.1. Introduction

In reality blood is a non-Newtonian fluid. It changes viscosity in dependence of the fluid properties and blood cell concentration. In the previous chapter blood was modeled as a Newtonian fluid, with a constant viscosity, whether in this chapter the viscosity change effects are included. Within a variety of viscosity models for blood two models, which describe the viscosity behavior during apheresis, have been chosen. Within these models viscosity is a function of the shear rate and the hematocrit. Further on the viscosity models are included in the computational code and simulations are performed. Simulations ran for three different geometry lengths and three different hematocrits. Thus effects of these two parameters on the separation process could be investigated. Within this model the viscosity changes. It is important to see how the viscosity changes and how strong the shear stresses are during the process. If the blood cells are exposed over a certain time to a critical shear stress, they are damaged and die. This process is called haemolysis. Due to that he investigation of shear stress is important to avoid haemolysis.

The non-Newtonian model is closer to reality, because it includes the complete behavior of blood. It includes the variable viscosity and this plays an important role in the separation process.

The main idea of this chapter is to have a model which simulates the process of apheresis, including all effects on density and viscosity. This model can then be applied on different geometries for parameter studies and finally aid the development of blood separators.

5.2. The viscosity model

Viscosity is resistance of a liquid to shear forces (and hence to flow). This property can be thought of as an internal friction. For a Newtonian fluid [128] the shear stresses $\tau$ are proportional to the velocity gradients, where the proportionality constant is the fluid viscosity $\mu$, as described in Equation (5.1).

$$\tau = \mu \frac{\partial u}{\partial y}$$

(5.1)
As for non-Newtonian models the viscosity change is dependent on the flow conditions. To describe the viscosity of a non-Newtonian fluid many models were developed.

The non-Newtonian behavior of blood is described by various models. The most known for physiological flow are the Casson [143], Walburn-Schneck [144] and Quemada [145-147] models. Due to the large hematocrit difference in the flow, these models are not well describing the viscosity during apheresis. Therefore other models for suspensions have been developed.

The first attempt to treat mathematically the viscosity of suspensions is by Einstein [148, 149], who derived for the viscosity of suspensions of rigid spheres the equation:

$$\mu_{\text{ suspension}} = \mu_{\text{ fluid}} (1 + kc)$$  \hspace{1cm} (5.2)

where $\mu_{\text{ suspension}}$ is the viscosity of the suspension, $\mu_{\text{ fluid}}$ is the viscosity of the pure fluid, $k=2.5$ for rigid spheres, and $c$ is the particle concentration by volume. A theoretical model for suspensions of rigid spherical particles as derived by Vand [150] has most often been used to model the viscosity of blood in centrifugal analysis. The Vand equation is an extension of the Einstein suspension viscosity equation [148, 149] and can be expressed in blood related nomenclature as

$$\mu_{\text{ blood}} = \mu_{\text{ plasma}} \exp\left(\frac{4.1H}{1.64-H}\right)$$  \hspace{1cm} (5.3)

where $\mu_{\text{ blood}}$ is the viscosity of blood, $\mu_{\text{ plasma}}$ the viscosity of plasma and $H$ hematocrit as defined in Equation (2.4). Although the Vand viscosity model has characteristics similar to blood, it does not correlate well to published data. In addition to hematocrit, the viscosity of blood is known to be dependent on shear rate, temperature, and plasma protein concentration [47, 151]. Numerous empirical models have been proposed [152], but none is as effective in modeling the behavior of centrifugal separation as the one introduced below

$$\mu_{\text{ blood}} = \mu_{\text{ plasma}} \beta \frac{\alpha H}{(1-H)^k}$$  \hspace{1cm} (5.4)

with $\alpha$ and $k$ are simple constants and $\beta$ is a shear sensitive term defined as

$$\beta = 1 + \frac{b}{n}$$  \hspace{1cm} (5.5)

where $b$ and $n$ are simple constants and $\gamma$ is the shear rate. The plasma viscosity as a function of the temperature is already defined in Equation (2.1). As for the plasma
viscosity $\mu_{37}$ at 37°C the value is set at 1.4 cp [50]. The constants and exponents of the Equations (5.4) and (5.5) can be determined from data reported in the literature. Data collected by Rand [48], Brooks [153] and Huang [130] have been used to define the constants of the model, which are $b=6.0s^n$, $n=0.75$, and $k=0.5$.

The Vand viscosity equation can also be approximated by the model of Equation (5.4) and provides some insight into the nature of the viscosity of blood. The concentration exponent $k$ is significantly higher for suspensions of rigid particles than for blood, but the concentration constant $a$ is similar. There are several important differences between the two types of suspensions. Blood consists of viscoelastic cells [151, 154, 155] and remains fluid at virtually complete packing. The viscosity of blood is sensitive to shear rate whereas suspensions of rigid particles generally remain Newtonian. Red blood cells elongate at higher shear rates [151, 152, 156] and when suspended in plasma, aggregate at low shear rates.

A more general model for the viscosity has been developed by Brown [54], by concatenating Equation (5.3) and Equation (5.4)

$$\mu_{\text{blood}} = \mu_{\text{plasma}} \beta (1-H) \exp \left( \frac{4.1H}{1.64-H} \right)$$

(5.6)

where the quantity $\beta (1-H)$ is artificially restrained to values much smaller than unity. The form of this viscosity model suggests that the streamlining effects of erythrocyte elongation is shear flow and directly dependent of the hematocrit. This model also includes shear rate effects without limitation. The effects near zero shear rates have been neglected, because the viscosity has a complete different behavior in a very low shear field [52, 157, 158]. A lower shear limit was set at 2.0.

The empirical model and Brown's model have been compared with experimental data [48, 153, 159], to check which of the two describes the viscosity behavior better. The models have been compared for different hematocrit values.

Brown's viscosity model fit very well for a hematocrit lower than 0.70. When the hematocrit exceeds the value of 0.70 the empirical viscosity mimics the viscosity behavior better. Thus the ideal model is a mixture of both, by taking the empirical model for a hematocrit over 0.70 and Brown's model for lower hematocrit.

5.3. The geometries

The geometry used for the simulations is the same as described in Chapter 4 by Brown [54] and Sartory [124]. It is a three dimensional bowl which is unfolded to a
two dimensional geometry. The 2-D geometry is mainly divided in three parts (Figure 5.1).

![Figure 5.1: The unfolded two dimensional geometry (data in mm).](image)

The inlet, which is the first part of the separator, has a length of 2.5 mm and a width of 1 mm. The second part is the main part where the whole separation process evolves. It is made of a smooth expansion which has an angle of 30°. The smooth expansion doesn’t allow the development of any instabilities, as it happens for flows in geometries with a sudden expansion [125, 160]. The middle part expands until it has a width of 4 mm which remains constant to the outlets. Three different lengths of the middle section, which are 13 cm, 16 cm, and 19 cm, are investigated to analyze the effect of the length. The middle section is split into two parts at the end. These two parts lead to the outlets, which have a length of 2.5 mm and a constant width of half a millimeter.

### 5.4. The computational model

The calculation scheme is the same as used in the simulation of the Newtonian model in Chapter 4.4. The flow field is first calculated with the commercial solver CFD-ACE, which solves the conservation equations at the center of each control volume within the solution domain. For the spatial discretization of the governing equations upwind, central and higher order methods have been tested. An algebraic multigrid technique is used for convergence acceleration and a SIMPLEC scheme [90] is used for the pressure-velocity coupling. Once the flow field is calculated the momentum equation for the particles is solved, as described in Chapter 4.4.2. Thus only the buoyancy, centrifugal and drag force are acting on a particle. The momentum equation is integrated twice over the time variable, using an implicit Euler scheme. The flow field information for the integration is obtained from the flow field solver.
When all particles are in their new position, the density and viscosity are calculated for each computational cell.

The density is calculated using the same scheme as described in Chapter 4.4.3. For every computational cell the hematocrit is calculated. Afterwards the density is calculated using Equation (4.5).

Viscosity is calculated using the empirical model (Equation (5.4)) or Brown’s model (Equation (5.6)). If the hematocrit in the cell is higher than 70% the empirical model is used, if it is equal to or smaller than 70% Brown’s model is used. The shear rates in the center of each computational cell are calculated by the flow field solver for the actual time step. Once the viscosity is calculated for every computational cell, it is spatially interpolated. A smoothed interpolation scheme [161-163] has been used. This procedure is needed to achieve convergence, due to the discrete hematocrit values between a computational cell and its neighbors. If viscosity is not spatially interpolated the flow field calculation would diverge, due to the discrete hematocrit difference between the computational cells. For further details on the accuracy and the properties of the interpolating functions the reader is referred to [162] and [164].

Once density and viscosity are calculated for every computational cell, they are set in the flow domain and the next time step begins. This procedure continues until the flow field reaches a quasi-steady state.

5.5. Simulation settings

5.5.1. The grids

For all geometries an unstructured triangular grid was constructed with the grid generator Gambit (Fluent Inc., Darmstadt, Hessen, Germany). The choice of an unstructured grid was made due to computational speed reasons. The speed of the computations with an unstructured grid over a structured grid was increased by a factor of four when implementing user written subroutines which interacted with the commercial code. The size of the grid elements varied between $3 \times 10^{-9}$ m$^2$ and $10^{-8}$ m$^2$. This corresponds to 54,700 grid elements for the shortest geometry to 67,900 grid elements for the longest geometry.

For grid independence studies of the model, two grids of differing refinement were created. To decrease the computation time, the grid independence study was performed on a different geometry, which is a tube with the length of 13 cm and a
width of 4 mm. This simple geometry is representative, because it simulates the separation process, which occurs in the center section of the real geometry. The inlet and outlet part are small compared with the length of the central part. Thus the choice of this geometry is valid for the geometry with the expansion. For grid independence studies of the model, two grids of differing refinement were created. The coarse grid was comprised of 33,000 elements and the fine grid had 60,000 grid elements. The refinement of the second grid was chosen so that one computational cell contains space for at least 10 representative particles. Thus the grid with 60,000 elements is the smallest grid for the representative particle size.

5.5.2. The simulation settings

To perform a comparison of the simulations with the experiments, the same simulation settings were used as in Brown’s experiments [54]. Brown performed experiments in a circular bowl (Figure 4.1) at a constant mid-slot radius of 7.02 cm, a chamber thickness of 4 mm and two different lengths of 13 cm and 43 cm. Most of the experiments were performed on the shorter bowl. The centrifuge was operated at rotational speeds of from as low as 1,425 rpm to as high as 3,250 rpm with most of the experiments conducted at 3,000 rpm. This corresponds to an acceleration between 159 to 803 g’s (1 g = 9.80 m/s²), although most of the experiments were conducted at 700 g’s. The blood flow rate at varied between 15 to 130 ml/min and the inlet hematocrit was adjusted from 0.26 to 0.52. These data were used to set the simulation conditions.

The computational domain rotates about an axis which is at a radial distance of 7.02 cm from the axis of symmetry of the separation device. The rotation speed $\omega$ is 314 rad/s, which corresponds to 3000 rpm. The viscosity of plasma is fixed at a value of 1.65 cp to calculate afterwards the local viscosity of blood, as the viscosity changes during the simulation. The density changes during the process and is calculated on the basis of the hematocrit in a computational cell. To accurately capture the transient behavior of the process, the time step is set at 0.1 seconds.

Uniformly mixed blood enters the inlet with a parabolic velocity profile of 0.01 m/s. This corresponds to an inlet mass flow of 30 ml/min. A constant pressure boundary condition is specified at the two outlets. At the walls a no slip condition is set.

The initial velocity is set in the entire flow domain at 0.005 m/s in the x-direction. At the beginning of the simulation the density is uniformly set at 1050 kg/m³ and the
viscosity at 3.1 cp. The flow calculation fully converges when it reaches a residual of $10^{-9}$ for the velocities and pressure at each time step.

5.5.3. The particle conditions

Each computational particle is not representing one blood cell but a certain number of particles (otherwise, prohibitively high numbers would be necessary). Therefore a representative number has been introduced. This number indicates the number of blood cells one computational particle represents. For this simulation the representative number was arbitrarily set to 10.

The initial and inlet hematocrit were fixed at 0.30 for the geometry with a length of 13 cm, 16 cm and 19 cm. On the smallest geometry two more simulations are performed with an inlet hematocrit of 0.30 and 0.40. Out of these values the initial number of blood particles was calculated, as listed in Table 5.1.

<table>
<thead>
<tr>
<th>Length / hematocrit</th>
<th>13 / 0.30</th>
<th>13 / 0.35</th>
<th>13 / 0.40</th>
<th>16 / 0.30</th>
<th>19 / 0.30</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. particles</td>
<td>313,000</td>
<td>361,000</td>
<td>418,000</td>
<td>386,000</td>
<td>458,000</td>
</tr>
</tbody>
</table>

Table 5.1: Number of blood particles in the different simulations.

The ranges of the parameter values of the blood particles are indicated as in Table 5.1 [19, 142]. The radius of the RBCs is 4 μm, for the WBCs 6 μm, and for the platelets 1.5 μm. The density of a RBC is set at 1100 kg/m$^3$, the density of a WBC at 1080 kg/m$^3$ and the platelets have the density of 1040 kg/m$^3$. The particles experience fully elastic collision with the walls. This is assumed because the time step $dt$ is small and the particle velocities near the wall are generally very small.

At the inlet the hematocrit is constant. Blood particles are introduced on a parabolic distribution. The inflowing plasma and blood cells have the same distribution profile. To improve the distribution of the blood cells, their parabolic distribution is moving slightly up and downwards. With this procedure, the blood cells are better mixed and the behavior is closer to reality.

5.6. Results

5.6.1. Grid independence

The simulation ran on a rectangular geometry, which is representing the center part of the separation chamber. Two simulations were performed on two different grids, a
coarse and a fine grid. The fine grid reaches the limitations set by the size of the blood particles, thus the finer grid is composed of 60,000 triangular grid elements. Grids containing cells physically smaller than blood particles would disturb the simulation results since the simulation procedure was developed with the Lagrangian particle approach. Comparing these two grids, it was shown, that the velocity distribution is nearly identical for both cases.

![Hematocrit profiles at three different cross-sections for the coarse (dashed line) and fine grid (dotted line).](image)

**Figure 5.2:** Hematocrit profiles at three different cross-sections for the coarse (dashed line) and fine grid (dotted line).

The particle distribution, respectively the concentration of the blood particles, does not change. Figure 5.2 shows, that the concentration distribution at three points of the geometry is practically identical for the fine and the coarse grid. The maximal difference of the concentration of particles is approximately one percent, while the mean difference of concentration of the two different grids is less than half a percent,
thus validating the grid independence of the solutions. Thus grid independence is valid [140, 141, 165].

5.6.2. Concentration of blood cells

Figure 5.3 shows the distribution of the RBC in the separator, when the flow reached the quasi steady state, for three different inlet hematocrits. The separation behavior changes with increasing the hematocrit. The packed cell bed builds up immediately after the expansion. It increases linearly until it is more difficult for the RBCs to settle, and the packed cell bed ceases to grow. For an inlet hematocrit of 0.30 this state is reached after a length of 8 cm. As for an inlet hematocrit of 0.35, it requires 9 cm and for 0.40 it takes more than 10 cm. Over the packed cell bed a fine layer with a lower RBC concentration is formed. Within this cell film, the concentration varies between 0.10 and 0.80. A higher inlet hematocrit corresponds to a larger RBC film over the packed cell bed. This phenomenon is very well shown in Figure 5.3. For the simulation with an inlet hematocrit of 0.30 the film is negligible, but it can be clearly recognized for the higher hematocrits. The top interface between the packed cell bed and the plasma has a wave-like shape. This is an effect of the oscillating inflow of the blood particles. They would, however, smoothen out if the residence time or chamber flow geometry were longer.

![Figure 5.3: RBC distribution for three different inlet hematocrits.](image-url)
The separators need some time to get from the initial uniform conditions to the quasi steady state. When the inlet hematocrit is 0.30 and the separator length 13 cm the calculation reaches the quasi steady state after 380 time steps, that corresponds to 38 seconds in a real separator. For the same separator with an inlet hematocrit of 0.35 this process requires 440 time steps, respectively 44 seconds. By increasing the hematocrit to 0.40 it needs 500 time steps, respectively 50 seconds.

Figure 5.4: WBC distribution for three different inlet hematocrits.

Within Figure 5.4 the separation pattern of the WBCs is depicted. Due to their low frequency the plots show mainly concentration centers. For the three cases shown, the flow patterns of the WBCs are looking very similar. They are diffused after the expansion. Thereafter they move towards the place where the centrifugal force is no longer acting on them, and they form a layer. For the three different cases this layer is formed after a length of 8.5 cm, 10.5 cm and 11.5 cm. Once the WBC layer is built, it moves towards the outlets. For an inlet hematocrit of 0.30 WBCs leave the separator only from the lower outlet while in the other two cases the outflow is split.

The platelet flow pattern of the three different cases is similar as shown in Figure 5.5. After the expansion the platelets are dispersed, as they would pass a diffuser. Just after the expansion they are uniformly distributed. Afterwards the particles in the upper
part are moving with the plasma towards the outlets. All the particles next to the separator’s bottom are drawn out of the high concentrated packed cell bed. In the separator center they build a region with a slight higher concentration. A second maximum is formed in the upper part of the separator. For the case with an inlet hematocrit of 0.30 these two maxima are lower than that from the other two cases. A higher inlet hematocrit corresponds to better developed maxima are developed, and a higher concentration.

![Platelet concentration graph](image)

**Figure 5.5**: Platelet distribution for three different inlet hematocrits.

The RBC concentration of the separators with different lengths is nearly similar in all three cases. As depicted in Figure 5.6, the packed cell bed is forming immediately after the expansion, grows and is formed after a length of 8 cm for all three lengths. After this length the hematocrit within the packed cell bed is over 0.80. The shape of the concentration distribution is not changing anymore. The longer the separator is the longer is the way of the packed cell bed, to reach the outlets.

A separator with the length of 16.5 cm and an inlet hematocrit of 0.30 needs 580 time steps, this corresponds to 58 seconds in a real separator, to reach a steady state behavior. These are 20 seconds, or 200 time steps, more as for the same hematocrit but a length of 13.5 cm. If the separator length is 19.5 cm this process needs 690 time steps, respectively 69 seconds.
**Figure 5.6:** RBC distribution for three different lengths at an inlet hematocrit 0.30

**Figure 5.7:** WBC distribution for three different lengths at an inlet hematocrit of 0.30
The shape of the WBC distribution is similar for three different separator lengths (see Figure 5.7). After the expansion they are uniformly distributed over the separator width. Moving towards the outlet they form a highly concentrated WBC layer. This layer becomes denser the closer the WBCs approach the outlet. With increasing separator length, the distance of this layer from the outlet decreases. The layer is located in the low concentration zone, where the packed cell bed has a hematocrit lower than 0.80.

Within the separator with a length of 19.5 cm the Platelets form two concentration maxima, moving towards the outlets (see Figure 5.8). The first concentration maximum, which is denser and wider, is in the separator middle and the second is the upper quarter. With decreasing separator length the higher maximum is decreasing and the lower increasing. The same shape has already been shown in Figure 5.5 for higher inlet hematocrit.

Figure 5.8: Platelet distribution for three different lengths at an inlet hematocrit of 0.30

Figure 5.9 shows the hematocrit of the different simulations over the separators width, just next to the outlets. The hematocrit distribution for the simulations with same inlet values is very similar. For cases with an inlet hematocrit of 0.30, the hematocrit
profiles are very well defined. The transition zone from zero hematocrit to the high concentrated packed cell bed is very small. The longer the geometry is, the smaller this zone is, and respectively the denser the packed cell bed is. The cases with higher inlet hematocrit show a larger transition zone. This transition zone is shown in Figure 5.9, where the hematocrit is varying between 0.10 and 0.80. The transition zone is shown as well in Figure 5.3 and Figure 5.6 as the low concentration film.

The shape of the WBC distribution next to the outlets is similar for all five cases (Figure 5.10). They are concentrated in one region with a maximum. The difference is in the height of the maximum and how wide this WBC zone is. A high inlet hematocrit leads to a WBC zone which is located towards the upper part of the separator. This zone is wider for the separation process with a low hematocrit. When the inlet hematocrit is 0.30, the WBC zone is in the lower third of the separator. Comparing the length of the geometry to difference can be observed. The WBC zone for an inlet hematocrit of 0.30 is wider and has a lower maximum as the long geometries. By increasing the length by 3 cm the, maximum of the WBC zone increases and the WBCs are less spread. When the separator’s length is increased by

![Hematocrit distribution next to the outlets](image)

**Figure 5.9:** Hematocrit distribution of the different simulations next to the outlets.
3 cm more, the maximum is still high but the WBC zone is pushed towards the lower third. Thus the effect of the length is that first the WBC zone gets more concentrated and afterwards is pushed towards the outer wall.

The platelet distribution over the width next to the outlets can be divided in two zones with two maxima, as depicted in Figure 5.11. One maximum of the platelet concentration is located next to the separator center. The second maximum is lower and is located in the upper quarter of the separator. This pattern is very visible for the simulations with an inlet hematocrit of 0.35 and 0.40. Next to y = 0 mm is a first maximum with a platelet concentration of 0.55% respectively over 0.60%. In the upper quarter of the separator a second maximum is reached where the concentration is over 0.2% respectively 0.4%. For the simulations with a higher inlet hematocrit these two zones are well recognizable. The pattern can be compared with the WBC distribution (Figure 5.10). That means that by elongating the separator a first time the concentration maxima increases and becomes more compact. By elongating the separator for another 3 cm the platelets are pushed toward the outer wall. The shortest geometry has a first maxima at y = -0.5 mm, which is wider and a second one at y =

**Figure 5.10:** WBC distribution of the different simulations next to the outlets.
1.4 mm. In the geometry with a length of 16.5 cm is more compact and has its maxima at $y = 0$ mm and $y = 1.2$ mm, but is compacter. When the length is increased to 19.5 cm, the maxima increase to 0.5% and 0.35%, and the entire concentration is pushed towards the bottom.

![Platelet distribution next to the outlets](image)

**Figure 5.11:** Platelet distribution of the different simulations next to the outlets.

5.6.3. Separation efficiencies

The separation efficiency is the basis for comparison between the results of the simulations and the experiments [54]. The separation efficiency is defined as the degree of elimination of any particular cell type from the packed cell bed at the outlet [54, 166, 167]. The analytical formulation is described in Equation (4.6).
Figure 5.12: Platelet separation efficiency plotted against plasma separation efficiency for the simulation and the experiments. The simulation were performed at an inlet hematocrits between 0.3 and 0.4, an inlet Reynolds number of 10 and a geometry length between 13 cm and 19 cm. The data indicate that platelets are swept out of the packed cell bed by the plasma for simulation and the experiments[54].

Figure 5.12 plots platelet against plasma separation efficiency, and as the graph indicates, the platelet separation efficiency tracks the plasma separation and confirms that platelets flow along with the plasma. The efficiency is calculated within the packed cell bed at the outlets. The single data points of the experiments are not attributed to any specific settings. The simulation data points were collected at 10 different heights at the outlets over ten time intervals. The computational simulations show that a high inlet hematocrit reduces the separation efficiency. They show as well the highest separation efficiencies for the longest geometry. Comparing the efficiency values of the experiments [54] and the simulations, the simulations predict a higher
plasma and platelet separation efficiency. The values in the experiments vary between 40% and 100%, while the prediction of the simulations is over 60%.

Figure 5.13 shows the WBC efficiency as a function of the hematocrit. The single data points of the experiments are not attributed to any specific settings. The process to obtain these points is the same as explained in Figure 4.7 and 4.8. The computational simulations show that a high inlet hematocrit reduces the separation efficiency. They show as well that the highest separation efficiencies corresponds to the longest geometry.

![Graph](image)

Figure 5.13: WBC separation efficiency is plotted against packed cell bed hematocrit at the outlets for simulation and experiments [54]. The simulation were performed at an inlet hematocrits between 0.3 and 0.4, an inlet Reynolds number of 10 and a geometry length between 13 cm and 19 cm. The data point appear to be clustered about low and high yields values.
This comparison reveals an explicable discrepancy between the experiments and the simulations. In the experiments two clusters of WBC efficiencies are recognizable, while the simulations show only one cluster of WBC efficiencies. In real blood, the WBCs can be separated in two groups with two different densities, but in the simulations the WBCs are one group of cells with one density. From this simplification, the simulations show only one cluster of data in the zone with a hematocrit between 0.75 and 0.90 and a separation efficiency over 80%. The experiments, however, show two clusters. The first cluster is in the zone with a hematocrit between 0.75 and 0.85 and a separation efficiency between 10% and 80%. The second cluster of the experiments lays in the zone with a hematocrit between 0.75 and 0.90 and a separation efficiency over 60%.

5.6.4. Shear stress and viscosity

![Shear stress for the three different inlet hematocrits.](image)

The shear stress distribution for the three cases with different lengths is similar (see Figure 5.14). At the inlet the shear stress reaches a maximum value of 0.02 N/m². After the expansion, the shear stress decreases and a shear stress distribution profile builds up. The distribution profile remains constant over the entire length. Next to the walls the shear stress is the highest and reaches a maximum value of 0.0125 N/m². At
the center of the separator the shear stress is equal to zero and slightly higher, due to
the very low shear rate.

![Shear stress distribution](image)

**Figure 5.15:** Shear stress for the three different lengths.

The shear stress distribution is similar for different separator length (see Figure 5.15). At the inlet the shear stress reaches a maximal value of 0.02 N/m². After the expansion the distribution remains nearly constant over the entire length. Next to the walls is a high shear stress zone with values which reach 0.0125 N/m² and in the center is a low shear stress zone, with values equal zero N/m² and slightly higher, due to the very low shear rate. Within the longest geometry the shear stress is increasing towards to the outlets at the bottom. After the central part the separated blood passes through the outlets, where the shear stress reaches similar values as at the inlet.

The variable viscosity feature differentiates the present non-Newtonian model from the work reported in De Gruttola et al. [65]. Figure 5.16 shows the viscosity in the separator for three different inlet hematocrit values. For an inlet hematocrit of 0.30 the viscosity distribution is divided into three regions. First the high viscous region which is mainly the packed cell bed zone. Within this zone the viscosity is between 7 cp and 8 cp. The second zone is the middle part where the viscosity is 5 cp. The third and smallest zone is located next to the top. Within here the viscosity is lower than 2.5 cp. Within this region the viscosity is slightly lower as the viscosity of blood. By
increasing the inlet hematocrit a fourth zone is generated. In the center of the separator, just after the expansion, a second high viscosity zone is generated with viscosity values between 7 cp and 8 cp. This zone grows with increasing inlet hematocrit.

\[
\text{viscosity}
\]

\[
\text{inlet hematocrit}=0.3
\]

\[
\text{inlet hematocrit}=0.35
\]

\[
\text{inlet hematocrit}=0.4
\]

Figure 5.16: Viscosity distribution for the three different inlet hematocrits.

In the separators with different lengths the viscosity profile is very similar (see Figure 5.17). It is divided into three zones. The high viscosity zone is the packed cell bed. In the center of the separator is a zone with a viscosity of 5 cp. Finally the top is a low viscosity zone, where the viscosity is lower than blood viscosity. When the geometry is elongated, some small secondary zones with high viscosity are generated next to the outlets.
5.7. Discussion and conclusions

Within this chapter it was shown that the blood separation process can be simulated through CFD using a non-Newtonian model. The method converges and delivers credible results. This model is a further development of the model used in Chapter 4, where the effect of the viscosity change has been neglected. In comparison with the previous model, this one includes the viscosity change and is closer to reality. The results are compared with published data [54, 124, 129].

5.7.1. The separation efficiency

Comparing the results of the simulations with the experimental data [54], one observes that they match well (see Figure 5.12 and Figure 5.13). The density difference between platelets and plasma is low and the centrifugal force does not act strongly on the platelets, generating separation efficiencies of plasma and platelets that are very similar. The experiments were performed with an inlet hematocrit which varied between 0.28 and 0.52, while the comparable CFD simulations used an inlet hematocrit in a narrower range. A higher inlet hematocrit lowered the separation efficiency. The low concentration film over the packed cell bed was larger, rendering
the separation of the blood cell types more difficult. Hence the experiments have a lower plasma and platelet separation efficiency.

The WBC separation efficiency graph shows two clusters of data for the experiments, but only one for the simulations (see Figure 5.13). In real blood WBCs exist as two groups with different densities [51]. Due to this density difference two clusters are present within the separation efficiency graph [54]. Within the simulations only one type of WBC was considered, leading to only one cluster of data. The efficiency is over 80% percent within a zone where the hematocrit varies between 0.70 and 0.90. WBC density corresponds to blood density with a hematocrit of 0.80. Thus the WBCs settle in this layer of the packed cell bed. The efficiencies of all experiments and simulations are included into the graph on Figures Figure 5.12 and Figure 5.13. The clustering effect is on account of the different simulation conditions. Comparing different geometry lengths with the same inlet hematocrit, the residence time of the particles is higher for a longer geometry, because the particles have more time to separate. The efficiency is lowered by increasing the inlet hematocrit because more blood cells have to settle. The residence time is the same but the higher particle concentration augments the increase in viscosity. Consequently, the flow resistance towards a blood particle increases. Hence a low concentration layer forms over the packed cell bed with increasing inlet hematocrit. Thus a larger blood viscosity effects a higher flow resistance for the settling WBCs, and the efficiency decreases.

5.7.2. The RBC concentration

The RBCs are the most frequent (95% of the hematocrit) and densest of all blood cells, and build a highly concentrated packed cell layer where the concentration exceeds 0.80 and no other cell types are present. This allows them to settle quickly at the outer separator wall, building a compact packed cell layer as shown in Figure 5.3, Figure 5.6 and Figure 5.9. With increasing inlet hematocrit a RBC film is generated over the packed cell bed. Hence the transition between the zero concentration zone and the packed cell bed becomes smoother. This is due to the length of the separator and inlet hematocrit. As more RBCs enter the separator, more time is necessary for the cells to settle. For the short geometry, the particle residence time is the same for all three cases of varying inlet hematocrit. Comparing the different geometry lengths, the transition from zero concentration zone to the packed cell bed becomes sharper, and the packed cell bed, compacter, while the low concentration film disappears. This
is due to the longer particle residence time. The packed cell bed experiences the centrifugal force over a longer time span, and becomes compacter.

5.7.3. The WBC concentration

The WBCs are building a high concentrated cell layer. This layer is located between the top of the packed cell bed and the RBC film (see Figure 5.4, Figure 5.7 and Figure 5.10). It is the region with a hematocrit of 0.80, where the local density is the same as the WBC density. Thus the centrifugal and buoyancy forces are comparable to one another, and only the drag force in the horizontal direction is acting on the WBCs. The layer forms due to two effects. From the bottom the WBCs are pushed out of the highly concentrated packed cell by buoyancy, and from the top of the separator the centrifugal force is pushing the WBCs towards the packed cell bed. A higher inlet hematocrit leads to a larger WBC layer, on account of the lower density difference and the higher viscosity, thus higher drag. When the WBCs are settling they have to pass through the low concentrated RBC film. Within this film, the flow resistance in this zone is large. Hence a higher inlet hematocrit requires more time for the WBCs require to settle. Comparing the effect of the length on the WBC layer, the WBC layer is less dispersed and more concentrated. The WBCs have more time to reach the zone with a similar density. Once the layer is compacted with the WBCs, the entire layer is pushed towards the outer wall, and becomes even more compressed. In this manner the WBCs are carried along with the 0.80 hematocrit zone towards the outer wall.

5.7.4. The platelet concentration

Platelet concentration is mainly divided into two higher concentrated zones (see Figure 5.11). The first zone is located within the center of the separator. Platelets are pushed out of the packed cell bed and moving towards the separator center. Thus the concentration increases. Because the higher velocity in the center and the lower centrifugal force, the platelets nearly do not settle. The higher concentrated zone is formed of the platelets which are just at the top of the separator. This region consists only of plasma and platelets. As well within this region the velocity is very low. The platelets are slowly pushed down. Thus the horizontal velocity increases in the flow field and the centrifugal force effect decreases. Hence, the platelets are moving towards the outlets and form a second maximum as shown in Figure 5.5, Figure 5.8 and Figure 5.11. A very low concentration of platelets remains trapped in the packed
cell bed which is acting as a porous medium, with high flow resistance, effectively trapping in them within the packed cell bed.

5.7.5. The shear stress and viscosity

Like for the shear stress as well the shape of the viscosity distribution is similar for all simulations. The viscosity increases at the bottom because of the high hematocrit. As described in Equation (5.4) and (5.6) dependent of the hematocrit and the shear rate. The hematocrit has a higher impact on the viscosity as the shear rate. Comparing Figure 5.16 and Figure 5.4 the shape of the RBC concentration and the viscosity distribution appear similar. This is due to the fact that shear rate is never reaching very low values. Thus the viscosity is only dependent of the hematocrit.

To avoid haemolysis during the separation process the blood cells should not be exposed to a shear stress over 150 N/m² for more three minutes [168-171]. The shear stress never reaches this critical shear stress. As well at the inlet and outlet zone were the shear stress is the highest, no haemolysis will occur. The cells are exposed to this overcritical shear stress over a time span of less than three seconds at the inlet and outlets. Due to the short exposure time and the low shear stress, there won’t be any damage to the blood cells [169, 171, 172].

The shear stresses are nearly identical in all simulations. Due to the same simulation conditions for all cases and the similar shape in the hematocrit distribution, as well the shear stress is not differing much between the single simulations. The shear rate and hematocrit are in a certain equilibrium state. When the hematocrit increases as well the viscosity increases and the shear rate decreases.

5.7.6. Improvement of the separation efficiency

To obtain a high efficiency of the separation process, the particle residence time has to be increased. This can be achieved by increasing the length of the separation chamber to retain the particles longer in the separator. Hence, the packed cell bed becomes more compact, because it is exposed over a longer time to the centrifugal field. The inlet hematocrit can be reduced by repeating the process sequentially. The hematocrit can also be reduced by mixing the inflow blood with some saline solution, which affects neither the blood properties nor the blood cells.
6. Discussion and Conclusions

A computational model and program which simulates the separation process of particles in a liquid has been developed. It is a mixed Lagrangian-Eulerian computation scheme. This computational model can be adapted on different types of fluids, particles and separation methods, e.g. centrifugation, sedimentation due to gravity. It also accounts for the variable viscosity of the fluid. The particle flow is calculated using a Lagrangian scheme. It can be adapted dependent on the separation method. As shown, with this model gravity including flocculation as well blood centrifugation can be reproduced. Due to the choice of an implicit Euler the integration is fast and stable. The time integration can be directly done without the need of any iteration steps. This scheme allows adding further effects to the process, e.g. flocculation.

6.1. Effect of the particle concentration on the flow field

Within a fluid with a low concentration of particles, the flow field is not affected by the particle flow. Thus the particle flow has not to be back coupled to the flow field solver. It is only necessary to calculate the flow field once. Afterwards the particles can just be integrated over the flow domain, using the flow field information. This leads to faster simulations and is very helpful to get fast results. This is very useful to optimize the design of separation devices, as described in chapter 4.

By increasing the particle concentration a back-coupling of the particle flow to the fluid is needed, even when the fluid has a Newtonian behavior. Within this work this happened by changing the fluid density dependent on the particle concentration. The density is directly related into the conservation equations, which are solved to calculate the flow field. Such a model can be used as well to model non-Newtonian fluids giving satisfying results [65].

Simulating non-Newtonian particle suspensions, its behavior can as well be taken in account. The back coupling is extended to the viscosity change using an appropriate viscosity model. Thus reality is approximated much more accurately. If viscosity related parameters need to be investigated it is important to include the non-
Newtonian behavior. As seen in Chapter 5 the viscosity change improves the accuracy of the calculation of the shear stress.

6.2. Comparison Newtonian to non-Newtonian model

Comparing the Newtonian and non-Newtonian simulations of the apheresis process the non-Newtonian shows much more accurate results, even tough the Newtonian model produces satisfying results. Non-Newtonian blood separation processes need more time to reach the quasi steady state. As the viscosity is adapted to the flow conditions the particle encounters a higher flow resistance. Hence the particles reach faster the quasi steady state. Whether in the Newtonian model the flow resistance is not changing. At the inlet blood is dispersed over the separator width. Due to the higher resistance in the non-Newtonian case, they move slower. Thus they cannot mix well into the packed cell bed next to the inlet. This leads to a higher efficiency. Once WBCs or platelets are in the high concentrated packed cell bed they encounter a high flow resistance. The packed cell bed has a similar behavior as a porous media. Thus the blood cells are trapped in it.

In the non-Newtonian model the WBCs and platelets, which are not in the packed cell bed, are moving in fluid with a lower density as it is for the Newtonian case. Therefore WBCs respectively platelet layer is formed. The platelets at the top of the separator are mainly moving only in plasma. Thus there the viscosity is similar to plasma viscosity and the flow resistance very low, whereas in the Newtonian model the platelets are moving in a fluid with higher viscosity. Due to this the drag at the top of the separators is low and the platelets can slightly move towards the bottom (see Figure 5.5 and Figure 5.8). This leads to a higher separation efficiency of the platelets for the non-Newtonian model. The differences between the Newtonian and non-Newtonian model shows that viscosity plays a key role in apheresis.

The non-Newtonian model allows more accurate calculation of the shear stress. As the shear stress is function of the viscosity, in the Newtonian model it is nearly impossible to get real values of it. If the shear stress is not known, no conclusions about haemolysis in the separator can be made.

6.3. Computational requests

Some user functions which are getting or setting information of the flow field are very time consuming. For a fine grid and a large amount of particles, as it the case for
blood, the computation needs a lot of time. The simulations were performed on a DEC-Alpha cluster consisting of eight 833 MHz and six 667 MHz 64-bit CPUs with a total of 20 GB of shared RAM. One simulation ran sequentially on one processor, hence no parallelization happened. The fastest simulation of the apheresis process, with 33'000 grid elements and 300'000 blood particles, was performed in more than three weeks. This problem could be avoided by optimizing the interaction ‘flow field solver – subroutine’. Therefore the access to the core of the commercial flow solver is needed. If this would be possible the computational speed can increase by a factor four to ten. Regarding the computational time, this would be a great improvement.

Recapitulating it can be said, specific separation processes have been modeled and a CFD model, which can simulate these processes, has been developed. These processes are simple gravity sedimentation to centrifugal non-Newtonian blood separation.
7. Literature


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