Stellingen
behorend bij het proefschrift *The Blending of Liquids in Stirred Vessels*
Ivo Bouwmans, 1992

Voor het berekenen van de totale energie die beschikbaar is voor het opbreken van een druppel zou niet de integraal genomen moeten worden over alle wervels die kleiner zijn dan de druppel\(^1\), maar de integraal over alle wervels met afmetingen in een gebied rond de druppelgrootte.

Het verlagen van de MAC-waarde voor cyclohexaan van 300 ppm naar 250 ppm\(^2\):\(^3\) suggereert ten onrechte een zeer nauwkeurige kennis van de gezondheidseffecten van deze stof en geeft daardoor een niet gerechtvaardigd gevoel van veiligheid.

Wegens de analogie met het gedicht van De Morgan\(^4\) zou de binnen het vakgebied van de stromingsleer vaak geciteerde tekst van Richardson over turbulentie volgens de oorspronkelijke versie\(^5\) aangehaald moeten worden: "... big whirls have little whirls that feed on their velocity, and little whirls have lesser whirls and so on to viscosity ..."

De opvattingen van Julian L. Simon\(^6\) gaan ten onrechte voorbij aan het risico van het optreden van onomkeerbare processen in de biosfeer.

De gebruikswaarde van dimensianalyse wordt buiten het vakgebied van de fysische technologie onderschat en daarbinnen overschat.

In navolging van het Engelse gebruik\(^7\) en dat van de rijksoverheid\(^8\) dienen Nederlanders in Engelstalige publicaties Nederland te vertalen met *The Netherlands*, inclusief lidwoord.

Het is onrecht dat de Technische Universiteit Delft, bij het ontbreken van een eenduidige wettelijke regeling en jurisprudentie in dezen, er stilzwijgend van uitgaat dat het auteursrecht van computerprogramma's die door promovendi tijdens hun promotieonderzoek geschreven zijn bij de Universiteit berust.

De term *houtvrij papier* dient vervangen te worden door *ligninevrij papier*, om het misverstand weg te nemen dat voor de produktie van deze papiersoort geen bomen gebruikt zouden worden.

Het promotiereglement van de Technische Universiteit Delft\(^9\) laat deze stelling toe.

---

3. "Health-based recommended occupational exposure limits for cyclohexane", rapport RA 15/90 van het Ministerie van SZW.
4. Augustus de Morgan, *"A Budget of Paradoxes"*, 1872 (zoals geciteerd in Jonathan Swift—*The Complete Poems*, Penguin, 1983): "Great fleas have little fleas upon their backs to bite 'em, / And little fleas have lesser fleas, and so ad infinitum."
5. L.F. Richardson, *"Weather prediction by numerical process"*, Dover Publications, 1922.
8. Buitenlandse Zaken, afdeling protocol buitenlandse missies.
THE BLENDING OF LIQUIDS IN STIRRED VESSELS
THE BLENDING OF LIQUIDS
IN STIRRED VESSELS

Proefschrift ter verkrijging van de graad van doctor
aan de Technische Universiteit Delft,
op gezag van de Rector Magnificus, prof. drs. P.A. Schenck,
in het openbaar te verdedigen
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Summary

In the process industries the blending of miscible liquids in the turbulent regime usually takes place in stirred vessels. For a long time there were two possible approaches to describing these processes. The 'engineering approach' combines measurements with dimensional analysis; the 'fundamental approach' concentrates on the underlying mechanisms of the blending process. In recent years the development of Computational Fluid Dynamics (CFD) has created new ways of analysis. The present study aims at combining the two approaches, using CFD, in order to arrive at a more generally applicable description of blending processes, in particular the blending of liquids of differing viscosities and densities.

Measurements were carried out with disc turbines and pitched blade turbines in vessels of 29 cm and 64 cm diameter, using a conductivity response technique and visualisations. The viscosity of the bulk was varied between 1 and 100 mPa·s, that of the addition between 1 and 5000 mPa·s. Density differences ranged from −100 (buoyant additions) to +400 kg/m³. The measurements show that when liquids of differing densities and viscosities are blended in stirred vessels, three mixing regimes can be distinguished.

- The stirrer controlled regime: liquid is added near the stirrer, or the bulk flow succeeds in transporting all of the added liquid to the stirrer. In this regime the dimensionless mixing time is equal to that of equiviscous, neutrally buoyant additions for added liquid viscosities between 1 mPa·s and 5 Pa·s (bulk viscosity 1 mPa·s): \(N^2 t_m \approx 30\). The dimensionless mixing time does not depend on the location of injection. In the turbulent regime this time is also independent of probe position. For small added liquid volumes the mixing time is independent of the added volume. When liquids of very high viscosities are added, long mixing times can result because the added liquid is insufficiently deformed by the high shear in the stirrer region.

- The gravity controlled regime: all of the added liquid rises to the surface or reaches the bottom of the vessel and remains there until it is blended into the bulk by turbulent vortices. When a high density liquid reaches the bottom, the resulting situation is analogous to that of a buoyant liquid surfacing. In this regime very long mixing times can result, depending on the viscosities of both phases as well as their density difference.

- The intermediate regime, between the other two regimes: only part of the added liquid is transported to the stirrer. In this regime the mixing time is unpredictable and can lie anywhere between the stirrer controlled mixing time and the gravity controlled mixing time. The mixing time depends on the amount of liquid that surfaces.

The probability of the added liquid surfacing or reaching the bottom is affected by the feed position, the density difference between the two liquids, their viscosity ratio and the stirrer speed. In the stirrer controlled regime this probability is negligible; in the gravity controlled regime it is 1. Small density differences may cause gravity controlled mixing, whereas small viscosity differences do not.

Low viscosity additions deform into sheets, whereas high viscosity additions deform into threads. This complicates the modelling of deformation, because as yet it is not clear which mechanism will prevail in a given situation.

Measurements with a Lightnin A310 impeller show that the energy needed for
homogenisation at equal stirrer speed, equal mixing time and equal power input is 0.36, 1.17 and 1.05 times that of the pitched blade turbine, respectively.

The absence of an influence of $\mu^*$ on the dimensionless mixing time in the stirrer controlled regime implies that the deformation of the added liquid is not the limiting factor in the blending processes in question. This is confirmed by visualisation experiments, which show that the deformation is fast. This, combined with the fact that $N_t \tau_m$ is constant, shows that when all of the added liquid is transported to the stirrer the homogenisation time depends on the rate of distribution of the added liquid over the vessel, as in the neutrally buoyant case. This means that the modelling of the mixing process can be divided into two parts:

1. Calculation of the probability of surfacing by calculating the trajectories of added fluid packages, taking into account buoyancy effects. A small probability indicates stirrer controlled mixing, a large probability indicates gravity controlled mixing.

2. Calculation of the time needed for distribution of the partly blended solute over the vessel by simulating conductivity measurements. Buoyancy effects and deformation can be neglected, because it can be assumed that the addition has been sufficiently merged with its direct surroundings.

In order to simulate these steps, a computer code, MIXIM (short for MIXing SIMulation) was written. It calculates the trajectories of added liquid packages, using the information about the three-dimensional flow field in the vessel that is supplied by the CFD program FLUENT. For each moment in time the next position of the addition is predicted using a probabilistic Monte Carlo method based on the local turbulent velocity. With these trajectories the probabilities of surfacing of buoyant additions and the time needed for distribution over the vessel of neutrally buoyant additions can be calculated.

The simulations show that the probabilities of surfacing for non-deforming drops depend on the feed position. Predicted probabilities that are high correspond to gravity controlled mixing in the experiments; low probabilities correspond to stirrer controlled mixing. The calculated value for the dimensionless stirrer controlled mixing time is equal to the measured value. Turbulence is essential for the mixing, but only up to a certain level. Above that level, a further increase of the turbulence intensity does not reduce the mixing time.

Circulation time distributions are bimodal and skew. Fluid elements that pass the stirrer plane but miss the stirrer cause the bimodality. The skewness enables long circulation times that in the case of high viscosity additions can give rise to mixing problems.

Although the flow in the stirred vessel is three-dimensional, the mixing characteristics are mainly affected by the axial and radial coordinate of the feed position. No correlation was found between the angular coordinate of a downward stirrer plane crossing and the angular coordinate of the next crossing; for the radial coordinate the correlation is very small. Simulation of a rectangular vessel of industrial size fitted with three impellers shows that the liquid flow is asymmetric and causes an asymmetric distribution of the probabilities of surfacing.

The modelling proposed in this thesis yields quantitative predictions about the blending in stirred vessels. The combination of observations and calculations offers the possibility of understanding more clearly the relevant mechanisms and their interaction.
Samenvatting

In de procesindustrie vindt het mengen van mengbare vloeistoffen in het turbulent regime doorgaans plaats in geroerde vaten. Lange tijd waren er twee mogelijke benaderingen om deze processen te beschrijven. De ‘technische benadering’ combineert metingen met dimensianalyse; de ‘fundamentele benadering’ richt zich op de onderliggende mechanismen van het mengproces. In de laatste jaren heeft de ontwikkeling van Computational Fluid Dynamics (CFD) nieuwe analysemethoden mogelijk gemaakt. Deze studie richt zich op een combinatie van de twee benaderingen, gebruik makend van CFD, om zo een meer algemeen toepasbare beschrijving van het mengproces te verkrijgen, in het bijzonder van het mengen van vloeistoffen met verschillende viscositeiten en dichtheden.

Met een geleidingsvermogensmethode en visualisaties werden metingen verricht in vaten van 29 cm en 64 cm diameter, uitgerust met schijfturbines en schuine-bladroorders. De viscositeit van de vatinhoud werd gevarieerd tussen 1 en 100 mPa·s, die van de toevoeging tussen 1 en 5000 mPa·s. De dichtheidsverschillen lagen tussen −100 (lichte toevoegingen) en +400 kg/m³. De metingen tonen aan dat, wanneer vloeistoffen met verschillende dichtheden en viscositeiten in vaten gemengd worden, drie mengregimes kunnen worden onderscheid.

* Het roederregime: vloeistof wordt toegevoegd bij de roeder, of de bulkstroming slaagt erin alle toegevoegde vloeistof naar de roeder te transporteren. In dit regime is de mengtijd gelijk aan die bij het mengen van vloeistoffen met gelijke viscositeit en dichtheid, voor toevoegingen met viscositeiten tussen 1 mPa·s en 5 Pa·s (bulkviscositeit 1 mPa·s): $N \cdot t_m \approx 30$. De dimensieloze mengtijd is niet afhankelijk van de injectiepositie. In het turbulent regime is deze tijd bovendien onafhankelijk van de sondepositie. Voor kleine volumes toevoeging is de mengtijd onafhankelijk van het toegevoegde volume. Wanneer zeer hoogviskeuze vloeistoffen worden toegevoegd, kunnen lange mengtijden optreden doordat de toegevoegde vloeistof onvoldoende vervormd wordt door de hoge schuifspanning in het roedergebied.

* Het zwaartekrachtsregime: alle toegevoegde vloeistof stijgt naar het oppervlak of zinkt naar de bodem van het vat en blijft daar totdat door turbulente wervels menging met de bulk plaatsvindt. Als een hoogviskeuze vloeistof de bodem bereikt ontstaat een situatie die analoog is aan die van een lichte vloeistof die het oppervlak bereikt. In dit regime kunnen zeer lange mengtijden optreden, afhankelijk van de viscositeiten van en het dichtheidsverschil tussen beide fasen.

* Het tussenregime, tussen de andere twee regimes: slechts een deel van de toevoeging wordt naar de roeder getransporteerd. De mengtijd in dit regime is onvoorspelbaar en kan elke waarde aannemen tussen die in het roederregime en die in het zwaartekrachtsregime. De mengtijd wordt bepaald door de hoeveelheid vloeistof die het oppervlak bereikt.

De kans dat de toegevoegde vloeistof het oppervlak of de bodem bereikt, wordt beïnvloed door de plaats van toevoeging, het dichtheidsverschil tussen en de viscositeitsverhouding van de twee vloeistoffen en het torerental. Deze kans is verwaarloosbaar in het roederregime, en gelijk aan 1 in het zwaartekrachtsregime. Kleine dichtheidsverschillen kunnen menging in het zwaartekrachtsregime veroorzaken, terwijl kleine
viscositeitsverschillen dat niet kunnen.

Laagviskeuze toevoegingen vervormen tot vlakken, terwijl hoogviskeuze toevoegingen vervormen tot draden. Dit bemoeilijkt de modellering van de vervorming, omdat het nog niet duidelijk is welk mechanisme in een gegeven situatie zal domineren.

Metingen met een Lightnin A310-roeder tonen aan dat de voor homogenisatie benodigde energie bij gelijk toerental, gelijk mengtijd en gelijk vermogen respectievelijk 0,36, 1,17 en 1,05 keer die van een schuine-bladroeder bedraagt.

Het ontbreken van een invloed van μ* op de dimensieloze mengtijd in het roerderregime betekent dat de vervorming van de toegevoegde vloeistof niet de beperkende factor is in de bestudeerde mengprocessen. Dit wordt bevestigd door visualisatiewachten, die laten zien dat de vervorming snel verloopt. Dit, samen met het constante getoon is van $Nt_m$, toont aan dat, wanneer alle toegevoegde vloeistof naar de roerder wordt getransporteerd, de homogenisatietijd afhangt van de verdelingsnelheid van de toevoeging over het vat, zoals in het geval van zwevende toevoegingen. Dit betekent dat de modellering van het mengproces in twee delen kan worden gesplitst.


2. Berekening van de tijd die nodig is om de gedeeltelijk gemengde toevoeging over het vat te verdelen, door geleidingsvermogensmetingen te simulieren. Drijfvermogen en vervorming kunnen worden verwaarloosd, daar aangenomen kan worden dat de toevoeging voldoende met de direct omringende vloeistof gemengd is.

Om deze stappen te simuleren werd een computerprogramma geschreven: MIXIM (een afkorting van MIXing SIMulation). Dit berekent de banen van toegevoegde vloeistofpakketjes, gebruik makend van de informatie over het driedimensionale stromingsveld in het vat door het CFD-programma FLUENT wordt geleverd. Voor elk moment wordt de volgende positie van de toevoeging voorspeld met een probabilistische Monte-Carlolomethode, gebaseerd op de lokale turbulente snelheid. Met deze banen kunnen de opdrikkans van lichte toevoegingen berekend worden, en de tijd die nodig is voor de verdeling van zwevende toevoegingen over het vat.

De simulaties tonen aan, dat de opdrikkans voor niet-vervormende druppels afhangen van de toevoegpositie. Grote voorspelde kansen corresponderen met het zwaartekrachtsregime in de experimenten; kleine kansen corresponderen met het roerderregime. De berekende waarde voor de dimensieloze mengtijd in het roerderregime is gelijk aan de gemeten waarde. Turbulentie is essentieel voor de menging, maar alleen tot een bepaald niveau. Boven dat niveau verlaagt een verdere toename van de turbulentie-intensiteit de mengtijd niet.

Circulatietijdverdelingen zijn bimodaal en scheef. Vloeistofelementen die het roerdervlak passeren maar de roerder missen veroorzaken de bimodaliteit. De scheefheid laat lange mengtijden toe die, in het geval van hoogviskeuze toevoegingen, mengproblemen kunnen opleveren.

Hoewel de stroming in het geroerde vat driedimensionaal is, worden mogenigeenschappen voornamelijk beïnvloed door de axiale en de radiale coördinaat van het toevoegpunt. Er is geen correlatie gevonden tussen de hoekcoördinaat van een neerwaartse doorkruising van het roerdervlak en de hoekcoördinaat van de volgende doorkruising;
voor de radiale coördinaat is de correlatie zeer laag. Simulatie van een rechthoekig vat van industriële afmetingen, uitgerust met drie roorders, laat zien dat de vloeistofstroming asymmetrisch is en een asymmetrische verdeling van de opduikkansen veroorzaakt.

De modellering die in dit proefschrift wordt voorgesteld levert kwantitieve voorspellingen op over het mengen in geroerde vaten. De combinatie van waarnemingen en berekeningen maakt een beter begrip van de relevante mechanismen en hun interactie mogelijk.
Chapter 1—Introduction

The problem of unpredictable mixing times in industrial mixing operations is introduced and the present research strategy using Computational Fluid Dynamics is outlined. The structure of this thesis is represented diagrammatically. The chapter is concluded with a summary of the project history.

1.1 Mixing in Industry and Research

In the process industries, mixing is performed in a wide variety of equipment on many scales ranging from small-scale laminar blending with static mixers to large-scale turbulent mixing with stirrers of several meters in diameter. The blending of miscible liquids in the turbulent regime, which is the subject of this thesis, usually takes place in vessels that are mounted with axial flow impellers, like a marine type propeller, a pitched blade turbine or a profiled impeller (e.g. Lightnin’s A310). Predicting to what extent a particular system from the wide range of stirrer and vessel geometries will produce the optimum mixing process in a given operation, is a question of knowledge of mixing process fundamentals. Insufficient understanding of mixing processes causes the continuous loss of a large amount of money in the chemical process industries (see Smith (1990)). Many processes, for instance in the petrochemical industries, but also in the food industry and in paint manufacturing, hinge on the blending of liquids of differing viscosities and densities. These differences can yield unexpectedly long mixing times, a situation that is undesirable in view of process planning and product quality control.

For a long time the only possible approach to a description of blending processes was founded on measurements and dimensional analysis. For the blending of liquids of similar physical properties this has led to an enormous amount of mixing time data and correlations for a huge number of possible combinations of stirrers and vessel geometries (see Tatterson (1991)). However, the literature about the blending of liquids with differing viscosities and densities is limited to processes that start with stratified layers. Moreover, it can provide information about specific individual mixing operations only, since in blending liquids that are dissimilar in these respects the number of parameters that can be varied is larger than in the case of similar liquids. A more fundamental approach is hampered by the complex flow structure in stirred vessels.

In recent years, however, the development of Computational Fluid Dynamics (CFD) has created new ways of analysis that are promising and challenging. The present study uses CFD to combine the ‘old’ method based on mixing time measurements with research on the underlying mechanisms of the blending process. These two methods offer different types of information and complement each other. The aim is to find the
causes of mixing problems following a more fundamental course and to arrive at a more generally applicable description of blending processes rather than to propose ad hoc solutions for selected mixing situations.

1.2 The Model

The model presented in this thesis uses the three-dimensional velocity field that is computed by the CFD program FLUENT to calculate, from a Lagrangian point of view, the trajectories that the added liquid will follow after injection into the vessel. In this way it is possible to predict, for instance, when mixing difficulties may arise with buoyant or settling additions and to predict important process characteristics like the mixing time.

In order to determine the effects of viscosity and density differences on the mixing time under turbulent flow conditions, measurements were made in laboratory scale vessels (29 and 64 cm in diameter). Viscosity ratios (added liquid viscosity divided by bulk viscosity) of 0.01 through 10^4 and density differences (added liquid density minus bulk density) of −100 through +400 kg/m^3 were used. It was found that buoyant and settling additions cause three mixing regimes, depending on the process conditions, the addition position and the properties of the liquids. In the stirrer controlled regime all of the added liquid is transported to the stirrer and blended in the same way as was found for equiviscous, neutrally buoyant additions. In the gravity controlled regime all of the added liquid rises to the surface (buoyant additions) or reaches the bottom of the vessel (settling additions) and remains there until it is blended into the bulk by the turbulent eddies. The intermediate regime lies between these two regimes: only part of the addition is transported to the stirrer. An overview is given in figure 1.1, which also shows the analogy between buoyant and settling additions.

Figures 1.2 through 1.4 give more detailed information about the examined situations. The figures show the sections that treat the measurements in oval boxes and those that treat the simulations in rectangular boxes. The measurements show that in the stirrer controlled regime the behaviour of buoyant and settling additions is the same as that of equiviscous, neutrally buoyant additions. This simplifies the modelling.

1.3 Structure of the Thesis

This introductory chapter is followed by a short literature review and a general outline of the proposed model. Chapter 3 contains the experimental results. The conclusions of that chapter lead to the model that is described in chapter 4. The results of the simulation program are presented and compared with the experiments in chapter 5. The structure of chapters 3 and 5 is indicated in figures 1.2 through 1.4 at the end of this
chapter. Finally, chapter 6 contains the general conclusions and some concluding remarks.

Parts of this thesis have been published before: the work by Smith & Schoenmakers (1988), carried out as a preliminary study to this project, and the work presented by Bouwmans & Van den Akker (1990). The chapters of this thesis will also be submitted for separate publication. Therefore, some of the information in this thesis is given in more than one chapter, so that each chapter can be read independently.

1.4 Project History

This project is a logical continuation of the work in the field of mixing in stirred vessels that has been undertaken at the Laboratorium voor Fysische Technologie of Delft University of Technology since its foundation in 1949. Kramers, the first professor, studied the mixing in stirred tanks using conductivity cells (e.g. Kramers & al. (1953)). Many studies followed, for instance by Holmes & al. (1964), who measured circulation times using the same technique, and Van Heuven (1969), who analysed liquid-liquid dispersions in stirred vessels. Van 't Riet (1975) explored the vortex system behind disc turbine blades with the use of a video camera rotating synchronously with the stirrer underneath a transparent vessel. Warmoeskerken (1986) used the same experimental arrangement and added new methods of analysis for the study of dispersing characteristics of turbine agitators.

This project, entitled 'Mixing of miscible fluids of differing viscosity', was initiated in 1985 by Professor John M. Smith D.Sc. It was accepted in the program of the STW (Stichting voor de Technische Wetenschappen—Netherlands Technology Foundation) in March 1986. The execution was given to the FOM (Stichting voor Fundamenteel Onderzoek der Materie—Foundation for Fundamental Research on Matter). Additional funding was supplied by Akzo International Research B.V. In December 1986 the Ph.D. work was started. At the end of that year Professor Smith left the laboratory for a new appointment as professor in Guildford, Surrey, UK. It was not until the beginning of 1988 that he was succeeded in Delft by Dr.ir. Harrie E.A. van den Akker, who renamed the laboratory Kramers Laboratorium after its founder.

The original subject of this study was the mixing of miscible fluids of differing viscosity. However, measurements showed that density differences have a more pronounced effect on the mixing time. Gradually the emphasis shifted towards the combined effect of density differences and viscosity differences. The advent of new computational methods enabled direct calculation of the flow field in the vessel and the simulation of the blending process. This finally led to the model presented in this thesis.

With this approach of using CFD techniques for the analysis of the blending process the present project falls in line with recent work by other authors. At mixing confer-
ences in Europe and America\(^1\), for instance, the number of computational studies that are presented is increasing. There is every indication that in the foreseeable future the computational approach will dominate mixing research. The role of experimental work will remain that of an indispensable source of information.

![Diagram](image)

**Figure 1.1.** Overview of the examined cases.
*More details are given in figures 1.2 through 1.4.***

\(^1\) The BHR (BHRA) and IChemE Mixing Conferences in Europe and the EF Mixing Conferences in America.
Figure 1.2. Simulation of neutrally buoyant additions. The numbers refer to the corresponding sections. An overview is given in figure 1.1.
Figure 1.3. Measurements with (ovals) and simulation of (rectangles) buoyant additions. The numbers refer to the corresponding sections. An overview is given in figure 1.1; figure 1.2 shows the neutrally buoyant case.
Figure 1.4. Measurements with (ovals) and simulation of (rectangles) settling additions. The numbers refer to the corresponding sections. An overview is given in figure 1.1; figure 1.2 shows the neutrally buoyant case.
Chapter 2—Outline of the Model

Two approaches found in the literature on blending in stirred vessels are discussed. A new method is proposed to simulate this blending process using Computational Fluid Dynamics (CFD) techniques. Using the CFD results, a separate program can then calculate, from a Lagrangian point of view, the trajectories of buoyant and settling drops added to the bulk, and estimate the mixing time. The outline of the method is given, together with an analysis of the single-phase flow in a vessel as calculated by the CFD program FLUENT.

2.1 Literature

In the process industries miscible liquids are often blended in turbulently stirred vessels. This study concerns the effects on these processes of viscosity and density differences between the addition and the bulk. The literature systematically dealing with these effects is limited to cases where layers of liquid are stratified at the beginning of the process (e.g. Van de Vusse (1955), Zlokarnik (1970) and Rielly & Pandit (1988)). In those situations the ratio between the added liquid volume and the bulk volume is comparatively large. In the process industries smaller quantities of liquid are often poured into the vessel while stirring is in progress. It is on these systems that the present work focuses.

While there is only a small number of papers devoted to this specific subject, the literature on the blending of liquids in general is extensive (see for instance Tatterson (1991)), and constitutes a valuable source of information. Two useful approaches contributing to a better understanding of mixing processes are found. The first uses dimensional analysis combined with measurements to find out which parameters determine the mixing time and to assess the power needed for homogenisation; the second attempts to arrive at a fundamental description of the blending of fluid elements in stirred vessels. Both approaches have their pros and cons. For the sake of convenience they will be labelled the engineering approach and the fundamental approach; in the following two sections these two approaches will be discussed in some detail. Subsequently, the model proposed in this thesis will be outlined.
2.1.1 The Engineering Approach

The engineering approach aims at structuring experimental results by means of dimensional analysis and it quickly yields practical correlations between dimensionless groups.

The much-cited paper by Hoogendoorn & Den Hartog (1967) is a representative example of this approach. The authors measure mixing times in several configurations using six stirrer types. One way in which they present the results of their mixing time measurements uses the dimensionless mixing time, $N\cdot t_m$ (where $N$ is the stirrer rotational speed and $t_m$ the mixing time). This represents the number of stirrer revolutions needed for homogenisation. The group is given as a function of the Reynolds number, $Re$, representing the ratio of inertia forces and viscous forces, which describes the flow conditions in the vessel:

$$Re \equiv \frac{\rho_0 N D^2}{\mu_0} \quad (2.1)$$

(where $\rho_0$ is the bulk density, $D$ the impeller diameter and $\mu_0$ the bulk viscosity). In the laminar regime (low values of $Re$), $N\cdot t_m$ is constant for a given vessel and stirrer combination. The same holds for the turbulent regime (high values of $Re$), but there the value of $N\cdot t_m$ is much lower than in the laminar regime. The constant value of the dimensionless mixing time implies that the number of stirrer revolutions needed to achieve homogenisation is constant. This means that in the laminar as well as the turbulent regime the stirrer can be seen as the 'clock' of the blending process: processes that are run at different stirrer speeds are identical when all times are made dimensionless using $N$. For values of $Re$ between the two regimes, however, $N\cdot t_m$ is not constant, and there is no similarity between processes run at different speeds.

In the literature, the dimensionless mixing time is sometimes multiplied by $D^3/V$, where $V$ is the vessel volume, to account for effects of the ratio of impeller diameter $D$ to vessel diameter $T$. This is only useful if systems with different $D/T$ ratios are to be compared, because otherwise the multiplication only shifts the results by a constant.

The dimensionless mixing time fails to give information about the energy needed for homogenisation, which is an essential factor in mixing operations. Hoogendoorn & Den Hartog obtain this information from power measurements. Their results are represented by means of the power number, $Po$:

$$Po \equiv \frac{P}{\rho_0 N^3 D^5} \quad (2.2)$$

(with $P$ the total power draw) as a function of the Reynolds number. In the laminar regime, $Po$ is inversely proportional to $Re$, whereas in the turbulent regime the power number is constant. Using this power number, the energy $E_m$ needed for the mixing process can be calculated by
\[ E_m = P_t_m = P_0 \rho_0 N^3 D^5 t_m. \]  

(2.3)

In order to include the power consumption and to eliminate the stirrer parameters \(D\) and \(N\), Hoogendoorn & Den Hartog introduce two dimensionless groups:

\[ \frac{P t_m^2}{\mu_0 T^3} = f \left( \frac{\rho_0 T^2}{\mu_0 t_m} \right). \]  

(2.4)

The argument on the right-hand side is a modified Reynolds number in that \(D\) and \(N\) have been replaced by \(T\) and \(1/t_m\). The term on the left-hand side can be interpreted as (Bouwmans & Van den Akker (1990)):

\[ \frac{P t_m^2}{\mu_0 T^3} = \frac{P}{\rho_0 T^3} \frac{1}{\nu_0} \frac{t_m^2}{\varepsilon} \frac{\varepsilon}{\nu_0} t_m = \frac{t_m^2}{t_K^2} \]  

(2.5)

where \(\nu_0\) is the bulk kinematic viscosity, \(\varepsilon\) is the energy dissipation rate per unit mass and \(t_K\) is Kolmogorov's time scale of turbulence. In this way the mixing time is measured in units of the smallest turbulent time scale. The groups can be used to choose the most efficient stirrer. To do this, however, \(t_m\) must be chosen in advance.

Zlokarnik (1967) also uses the groups introduced by Hoogendoorn & Den Hartog and adds a new relation:

\[ \frac{\rho_0^2 P T}{\mu_0^3} = f \left( \frac{\rho_0 t_m^3}{\mu_0 T^2} \right). \]  

(2.6)

In this case, the group on the left can be interpreted as:

\[ \frac{\rho_0^2 P T}{\mu_0^3} = \frac{P}{\rho_0 T^3} \frac{\rho_0^3 T^4}{\mu_0^3} \frac{\varepsilon}{\nu_0} T^4 = \frac{T_A}{t_K} \]  

(2.7)

where \(t_K\) is Kolmogorov's turbulent length scale. Zlokarnik's groups have the same disadvantage as those of Hoogendoorn & Den Hartog: \(t_m\) must be chosen first.

In a later paper Zlokarnik studies the influence of density and viscosity differences on mixing times (Zlokarnik (1970)), and uses the Archimedes number, which contains \(\Delta \rho = \rho_a - \rho_0\), the density difference between added liquid density \(\rho_a\) and bulk density \(\rho_0\):

\[ Ar \overset{\text{def}}{=} \frac{\Delta \rho g D^3}{\nu_0^2 \rho_0}, \]  

(2.8)

(where \(g\) is the gravitational acceleration). This number weighs the buoyancy forces acting on the added liquid against the viscous forces in the surrounding liquid. Zlokarnik arrives at the following relation for paddle stirrers (turbulent regime for \(Re > 10^2\)):

\[ \frac{\sqrt{N t_m}}{Ar^{1/3} + 3} = \frac{51.6}{Re}, \quad \begin{bmatrix} 10^1 < Re < 10^5 \ \\ 10^2 < Ar < 10^{11} \end{bmatrix}, \]  

(2.9)
Chapter Two

Zlokarnik shows this relation to be valid for a range of liquid properties, but does not clarify the meaning of the term on the left. For $\Delta \rho \rightarrow 0$ (so $Ar \rightarrow 0$), the relation does not hold, for in that case $N\cdot t_m$ should become independent of $Re$. This approach has not been adopted by later authors.

The group commonly used to account for buoyancy effects is the *Richardson number*, as in Rielly & Pandit (1988):

$$Ri \overset{\text{def}}{=} \frac{\Delta \rho g H}{\rho_0 N^2 D^2}$$  \hspace{1cm} (2.10)

(with $H$ the liquid height in the vessel). This number is a measure for the ratio of the potential energy density needed to pull the added liquid into the stirrer and the kinetic energy density of the bulk. Whereas the Archimedes number contains static parameters only, $Ri$ includes the operating parameter $N$, and can therefore be used as the independent variable.

The engineering approach quickly yields useful empirical correlations for individual systems, while dimensionless groups clearly illustrate the differences in behaviour between the various mixing conditions. For that reason dimensionless groups will be used for the presentation of the mixing time measurements in chapter 3. However, new measurements are needed for each new combination of vessel geometry and stirrer type, liquid properties and feed position. Moreover, it does not become clear what mechanisms underlie the mixing process, because the vessel is treated as an integral system rather than analysed into constituents. It is doubtful, therefore, whether the dimensionless groups that are found could contribute to a better fundamental understanding and description of the mechanisms in the mixing process, which is the major object of this study.

2.1.2 The Fundamental Approach

The fundamental approach concentrates on the underlying mechanisms of the blending process. The theories describing these mechanisms can be used as building blocks for the description of more complex cases. Firstly, we will consider the literature that focuses on the blending of miscible liquids of about equal physical properties. Then the literature that deals with the effects of viscosity differences and the literature on buoyancy effects will be treated.

*The Blending of Liquids of about Equal Viscosities*

An important part of the literature concerns the blending of miscible liquids of about equal physical properties that contain fast reacting chemicals. In that situation the
mixing rate determines the final product composition. Attention centres on molecular diffusion accompanied by fine-scale, laminar fluid deformation: the micromixing (Bourne & Dell'Ava (1987)). Ottino (1982 & 1989) gives a thorough analysis of this deformation for several types of idealised flow. The analysis concerns the combined deformation and diffusion in configurations of layers of liquid with alternating concentrations of a marker substance (see figure 2.1). These configurations result from the motions of the turbulent vortices: rotation and vortex stretching (see figure 2.2). Bourne and collaborators analyse simple shear fields (Angst & al. (1982)) and extensional flow (Bolzern & Bourne (1983)), simulating fast competitive, consecutive reactions. Baldyga & Bourne (1988) incorporate the spatial distributions of velocity and energy dissipation rate using a simplified flow model of the vessel. They obtain satisfactory agreement between predicted and observed results of product distributions.

![Figure 2.1. Layers of liquid of alternating marker concentration.](image)

![Figure 2.2. Vortex motion resulting in alternating layers of liquid.](image)

*The Effect of Viscosity Differences*

In the majority of cases where non-reacting liquids of differing viscosities are blended the concept of micromixing is not applicable for two reasons.

1. In systems with viscosity and density differences the flow within the added liquid differs from the flow in the bulk. Therefore, contrary to situations in which the liquids to be blended have equal viscosities, the theories about deformation and stretching of the bulk flow cannot be used to predict the deformation and stretching of the addition.

2. Visualisation and mixing time measurements demonstrate—as will be shown in
the next chapter—that the deformation of the added liquid is fast enough to neglect the time needed to merge the addition with its direct surroundings. In that case the addition can be assumed to have the same properties as the bulk liquid, and the mixing time will be that of equiviscous, neutrally buoyant additions. The mixing time then equals the time needed for the homogeneous distribution of the addition over the vessel, the macromixing. This is confirmed by the empirical fact that $N_{c}t_{m}$ is constant, which shows that the bulk viscosity is not important, unlike in micromixing situations.

In addition, with non-reacting liquids there is no need for a blending process on molecular scale. The only requirement is that all containers used for further distribution of the product (e.g. paint, oil) contain the same amount of all components. The process is therefore monitored by means of sampling on a scale that is large compared with molecular dimensions.

Information about the effect of viscosity differences on the deformation of liquids is limited. The velocity field and the deformation can only be calculated for simple flows and geometries. For example, the stretching of thin viscous inclusions in Stokes flow is treated by Wilmott (1989). De Bruijn (1989) studies the deformation of immiscible drops in simple shear flow. He calculates the shape of drops in time-dependent flows. The systems have viscosity ratios between 0.5 and 5. However, the complexity of the turbulent flow in stirred vessels does not allow the use of these methods.

*The Effect of Density Differences*

The relative motion of particles and drops due to buoyancy has also been studied in simple systems only. Even for solid spheres and spherical drops the theories are incomplete and rely heavily on empirical data. Wallis (1974) gives a survey of the correlations that have been found for several conditions. These include the cases where drops are deformed by the effect of buoyancy itself, but there are no relationships for the rising velocities of drops that are deformed by velocity gradients in the surrounding liquid.

In general, a more fundamental approach is only possible in idealised systems. The models mentioned above offer possibilities for extension to more complicated flows. However, the use of these models for stirred vessels is hampered by the existence of a wide variety of flow types in various regions of the vessel. Application of the models is only possible if the path that an added fluid element will follow can be predicted. The model proposed here uses Computational Fluid Dynamics to do this.
2.1.3 The Proposed Model

The model proposed in this study tries to strike a balance between the engineering and the fundamental approach. Mixing time measurements and visualisation in stirred vessels have shown (see the next chapter) that the paths followed by the added liquid determine the mixing time. For instance, the stirrer distributes the added liquid over the vessel, which yields a constant value of $N \cdot t_m$; however, when buoyancy forces dominate, some of the added liquid reaches the surface, and the addition is blended into the bulk by an altogether different mechanism, which can yield very long mixing times. It is difficult to predict which mechanism will dominate. This situation is not easily grasped even by a combination of dimensionless groups. Therefore, a method has been developed that enables the calculation of the paths the added liquid follows. These paths can now be predicted with Computational Fluid Dynamics (CFD). This technique gives information about the flow field that was not available until very recently.

Computational Fluid Dynamics is a general term for the branch of computer science that is dedicated to the simulation of fluid flows. CFD programs are able to calculate the flow fields for many types of flow. This is done by solving the mass and momentum balances iteratively for a large number of control volumes until these balances meet a chosen criterion.

The use of CFD to make predictions about mixing equipment is growing fast. Mann & Mavros (1982) and Baldyga & Bourne (1988) use estimated two-dimensional flow fields for the prediction of mixing characteristics. Their predictions, although not based on calculation of the whole flow field, are a good approximation of reality. Ranade & Bourne (1991) and Bakker (1992) use the calculated three-dimensional flow field to make predictions about blending and gas dispersion, respectively. Their results show that three-dimensional calculations give an even better prediction about the processes.

The model proposed here also uses the results of three-dimensional flow calculations. Figure 2.3 shows the procedure of the modelling. Mixing time measurements give information about which parameters are important under what conditions. The models found in the literature, dealing with such matters as the relative velocity of the added liquid due to buoyancy effects and the turbulent velocities, can be used as sub-models for the more complex case. These sub-models are combined in a computer program, MIXIM (short for MIXing SIMulation). MIXIM simulates the mixing in a vessel by calculating the added liquid’s path through the vessel, starting at a chosen feed position. This is done from a Lagrangian point of view. Until very recently, the Eulerian approach was more common (e.g. Ranade & al. (1991)). It treats the computational cells as completely mixed for the calculation of the marker concentration. For continuous processes like gas-liquid dispersion (Bakker) the Eulerian approach is to be preferred. For batchwise processes, however, the blending should preferably be modelled from a Lagrangian viewpoint, as by Baldyga & Bourne.¹

¹It is interesting to note that the Lagrangian description is actually also due to Euler (Ottino (1989)).
On the basis of the calculated paths, predictions about the mixing process can be made, for example the mixing time. MIXIM obtains the information about the local velocities in the vessel from output files of the CFD program FLUENT that calculates the three-dimensional flow field. FLUENT in turn gets the information it needs for the calculation of the flow field from Laser Doppler Velocimetry (LDV) measurements in a vessel. This procedure enables the prediction of mixing times for a wide variety of process conditions.

2.2 CFD Calculations

In order to arrive at the correct flow field using CFD, the right boundary conditions should be fed into the computer. The stirrer boundary conditions are necessarily based on measurements: as yet, FLUENT is unable to model the stirrer explicitly. Furthermore, for turbulent flows it is necessary to choose an appropriate closure model for the Reynolds stresses that predicts the momentum transport by turbulent eddies (see Rodi (1984)). For the sake of concision, only the necessary data are given here. The velocity measurements and CFD calculations were carried out by Bakker during his Ph.D. project at the Kramers Laboratorium, Delft. More details than given here can be found in his thesis (Bakker (1992)).
2.2.1 Velocity Measurements

For the present work, the flow field in a vessel stirred by a Pitched Blade Turbine (PBT) was calculated by the CFD program FLUENT. The first step in the process is the acquisition of boundary conditions that can be used for the flow field calculations. It was assumed that the time-averaged values of the mean and turbulent (root mean square) velocities in the impeller discharge flow are necessary and sufficient in order to calculate the total flow field in the vessel (see also Ranade & Joshi (1989)). These velocities were measured using a two-dimensional TSI fiberflow Laser-Doppler system. A 44 cm vessel mounted with a PBT was used. All measured velocities \( u \) (mean and rms values) were scaled, using

\[
\frac{u}{ND} = \text{constant},
\]

(2.11)

to a geometrically identical vessel of 64 cm, the size of one of the vessels that were used in the mixing time measurements. This scaling rule can be assumed to be valid for the small scale-up factor that is used here. The scaling of the flow field will also be treated in the section on the mixing simulation program (section 2.3). The scaled values were used as boundary conditions for the FLUENT calculations.

2.2.2 Calculation of the Flow Field

FLUENT version 3.02 was used for the flow calculations. The turbulence was simulated using the algebraic stress model (ASM), modelling anisotropic turbulence, because the ASM results fit the experimental data better than the results of the \( k-\varepsilon \)-model do (Bakker (1992)). The large differences in the turbulent velocity components also show that an anisotropic model is required.

The flow was calculated on a non-uniform grid of 20328 (42×22×22) cells for a cylindrical vessel and on a uniform grid of 24200 (22×22×50) cells for a rectangular vessel. The measured axial and tangential velocities were prescribed at the lower boundary of the impeller, as presented by Bakker. Because the radial velocities could not be measured, the turbulent kinetic energy per unit mass, \( k \), was estimated by

\[
k = \frac{3}{4} \left[ u_1'^2 + u_3'^2 \right],
\]

(2.12)

with \( u_1' \) and \( u_3' \) the axial and tangential turbulent velocities, respectively. The local energy dissipation rate under the stirrer, \( \varepsilon \), was calculated assuming that the turbulent length scale was proportional to the width of the impeller blades \( W_b \) (Wu & Patterson (1989)):

\[
\varepsilon = 0.25 \frac{k^{3/2}}{W_b}.
\]

(2.13)
The power law interpolation scheme was used to solve the equations. Calculations with the QUICK\(^2\) scheme, also provided by FLUENT, did not converge in all cases. Moreover, QUICK is slow, so the power law scheme was chosen for further calculations.

The calculation was assumed to be converged when the sum of the normalised residuals was smaller than \(10^{-3}\). Calculations of similar cases showed that decreasing the criterion to \(10^{-5}\) does not change the predicted flow field.

For verification of the calculated velocities, axial velocities were measured at various positions in the 44 cm vessel. The predicted values corresponded satisfactorily to the actual values (Bakker).

### 2.2.3 One-Phase FLUENT Output

Measurements and FLUENT simulations show that the average velocity field in a baffled vessel is three-dimensional in character. This means that the observed phenomena will not only depend on the distance from the axis and the depth in the vessel, but also on the angle with regard to the baffles. The same holds, of course, for non-circular vessels, independent of the presence of baffles.

The 64 cm vessel used for mixing time measurements will be analysed here as an example. The geometry of the cylindrical vessel is given in figure 2.4. The vessel is filled with water; the PBT speed is \(1 \text{ s}^{-1} (Re = 6.5 \times 10^4)\).

![Figure 2.4. Geometry of the mixing vessel.](image)

\(^2\) Quadratic Upstream Interpolation for Convection Kinematics.
Figure 2.5. Axial & radial velocities in a plane just in front of a baffle, as calculated by FLUENT.

Figure 2.6. Axial & radial velocities in a plane midway between two baffles, as calculated by FLUENT.

Figure 2.5 shows the calculated axial and radial velocity components in the plane just in front of a baffle. This flow most closely corresponds to the intuitively expected pattern of a single large circulation loop. This pattern has dominated the ideas about the PBT-stirred vessel for a long time (e.g. Beek & Muttzall (1975), Mann & Mavros (1982) and Baldyga & Bourne (1988)). In figure 2.6 the plane halfway between two baffles is given. In this plane almost all liquid close to the surface flows downwards. These two figures illustrate the three-dimensionality of the mean flow. The most recent literature does include three-dimensional calculations (e.g. Ranade & al. (1991) and Bakker (1992)).
The radial and tangential flow components in the plane 16 cm below the liquid surface are shown in figure 2.7. A large vortex behind the baffle can be seen. Figure 2.8 shows a much smaller vortex in the plane about 7 cm below the impeller.

The data provided by FLUENT include the dissipation rate per unit mass, $\varepsilon$, and the turbulent kinetic energy per unit mass, $k$. These parameters will be used for the simulation of the turbulent component of the velocity. Both parameters are very inhomogeneously distributed. For the case under consideration, FLUENT predicts local values of $\varepsilon$ between $3 \times 10^{-6}$ and 0.5 W/kg, with a volume weighed average of $4 \times 10^{-3}$ W/kg. Because of its low dependency on $\varepsilon$, the Kolmogorov length scale, $l_K$, varies only between $4 \times 10^{-5}$ and $7 \times 10^{-4}$ m. The kinetic energy ranges from $2 \times 10^{-5}$ to $3 \times 10^{-2}$ J/kg, average $3 \times 10^{-3}$ J/kg. All values for the parameters given here depend on the grid: larger cells yield averages over larger areas. Therefore, the values should be viewed as examples only.

It should also be noted that the stirrer is not modelled explicitly by FLUENT, so the maximum predicted values of $\varepsilon$ and $k$, and therefore the minimum value of $l_K$, are not reliable. For the stirrer a separate model must be used until computational power is strong enough to model the stirrer completely.

Moreover, the total power draw predicted by FLUENT is less than the measured value. This is partly due to the omission of the stirrer from the model, but even if that is corrected, the predicted power consumption is still a little lower than it should be (Bakker).
The character of the flow was not modelled fully, as the time-dependence of the mean flow was not taken into account. The mean flow exhibits slow fluctuations at a scale between the vessel diameter and the smaller turbulent eddies. This behaviour should be included in the flow model, for it can add to the mixing problems. The chance that the added liquid will reach the surface increases if the liquid is added at a moment when the axial flow is upward.

Therefore, a complete description of the phenomena observed in the vessel will not be acquired until four-dimensional flow calculations—including time—are carried out. The calculations presented in this thesis are three-dimensional owing to computational constraints. It is to be expected that in the near future computational speed will increase to a level at which full four-dimensional calculations will be possible in practice.

2.3 Mixing Simulation Program—MIXIM

This section outlines the basic principles of the Pascal computer code MIXIM, which was developed for the final calculations of the mixing characteristics, and explains the advantages of MIXIM over FLUENT's option for the calculation of particle trajectories. In chapter 4 the models and the program MIXIM will be discussed in more detail.

MIXIM uses a probabilistic Monte Carlo method to model the mixing process. The added liquid is assumed to enter the bulk as a spherical drop. It is also assumed that the added liquid has no influence on the bulk flow. This assumption is valid for relatively small amounts of added liquid. The drop's trajectory is calculated from a Lagrangian viewpoint: for each time step the next position of the drop is determined from the turbulent bulk velocity combined with the drop's buoyancy velocity. In order to do this, MIXIM uses the local values of the mean velocity, the energy dissipation rate, and the kinetic turbulent energy, as calculated by FLUENT.

With the calculated trajectories it is possible to predict when the addition will be likely to reach the surface or the bottom of the tank. It is also possible to calculate the circulation time (the time between two stirrer passages) and the mixing time (the time needed for the homogenisation of the vessel contents). This mixing time is found by tracking a large number of drops and registering the number of them that passes a chosen area, the 'probe', as a function of time. In this way a conductivity measurement (see chapter 3) can be simulated.

The FLUENT flow field calculated for the 64 cm vessel was scaled by MIXIM in order to simulate the mixing in a 29 cm vessel. This was done by keeping

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3 In the literature on miscible liquids the word *drop* is frequently used to indicate parts of the added liquid. In that case, as in this thesis, the word implies neither immiscibility nor the presence of interfacial tension.
\[ \frac{u}{ND} \quad \text{and} \quad \frac{\varepsilon}{N^3 D^2} \]

constant \((k \text{ scales with } u^2)\). This assumption is only valid on condition that the flow field scales with the macroscopic parameters. As the flow in the vessel is turbulent, viscous effects can be assumed to be negligible and the condition is met.

The calculation of the paths followed by particles in the vessel can also be done using the particle tracking facility supplied by FLUENT. However, MIXIM has some advantages over this standard facility. The drop diameter and addition point can be changed more flexibly: the program can analyse an array of positions and diameters. Moreover, with MIXIM the response of a conductivity cell can be simulated and circulation time distributions can be calculated. Finally, in order to analyse the flow field using FLUENT at different stirrer speeds and vessel scales the whole flow field must be calculated again for each scale and speed. The calculation by FLUENT of a flow field in each of the vessels under consideration took more than a week. The main reason for this long calculation time is the absence of a gap between the baffles and the vessel wall. The resulting circulation loops behind the baffles exhibit a slow computational convergence (see also Bakker (1992)).

2.4 Conclusions

In the literature on mixing in stirred vessels two lines of approach are found. The engineering approach combines dimensional analysis with measurements. The fundamental approach aims at a description of the fundamentals of the blending process, mostly by studying idealised flows. This project attempts to use a combination of both methods, complemented by information gained from recent developments in Computational Fluid Dynamics. The method of working involves the successive application of flow measurement by laser doppler anemometry, CFD flow calculation by FLUENT and flow analysis by the program MIXIM.

In principle, the procedure described here can be used for any vessel size and geometry, which would facilitate equipment design and scale-up. Until recently, the mixing process could only be analysed experimentally. This resulted in a large number of correlations, as reviewed by Tatterson (1991). With the computational methods it is now possible to study, for instance, the effect of \(D/T\) ratio, impeller to bottom clearance, or baffle configuration on the average mixing time and its deviation, or on the circulation time. Moreover, the chosen model enables a better understanding of the interaction of the mechanisms that underlie the blending process, because the individual
effects of the mechanisms can be simulated. For instance, the density difference or the turbulence intensity can be changed to values that are impossible in a real situation, so the extreme effects of these changes can be studied.

More reliable bulk flow calculations and a better understanding of the small-scale processes will eventually lead to more reliable predictions of the mixing characteristics. Although the need for experiments will decrease, measurements will remain essential for verification purposes.
Chapter 3—Measurements

Mixing time measurements were carried out in turbulently stirred vessels with miscible liquids of differing viscosities and densities. Depending on the flow characteristics and liquid properties three mixing regimes can be defined for buoyant additions: the stirrer controlled regime, the gravity controlled regime and the intermediate regime. Settling additions exhibit analogous behaviour. In the stirrer controlled regime the dimensionless mixing times are equal to those for liquids of equal properties (about 30), the gravity controlled values can be much higher. In the intermediate regime the dimensionless mixing times can be anywhere in between.

3.1 Introduction

This study is concerned with the turbulent mixing of miscible liquids in stirred tanks. Traditionally, visualisation and mixing time measurements are very important sources of information about the processes involved. The literature on these subjects is vast (see for instance Tatterson (1991)), mainly because the number of independent variables is large. Each combination of vessel geometry, stirrer type, liquid properties and liquid addition method can be expected to behave differently.

The studies reported in the literature on the mixing of liquids of differing viscosities and densities are concerned with set-ups in which the process is started with stratified layers. The ratio of the added liquid volume to the bulk volume is comparatively large in those situations. Industrial procedures often involve the addition of smaller quantities of liquid during operation. The present research project centres on the type of system in which the additions consist of small quantities of liquid with viscosities and densities that differ from those of the bulk.

In the work by Smith & Schoenmakers (1988), which was carried out preliminary to this project, experiments were carried out with high viscosity additions in water, because differences in mixing times were expected in that situation. Later series of experiments involved aqueous additions to more viscous bulks. During extended measurements it became clear that density differences are more likely to cause longer mixing times than viscosity differences are (Bouwman & Van den Akker (1990)). New series of experiments then proved the dependence of mixing time on a combination of viscosity and density differences.

In this chapter the experimental method is discussed first. Then the measurements with buoyant additions are presented, followed by those with settling additions.
3.2 Experimental

In the course of the project several experimental setups and two methods of data processing were used. The common features will be discussed in this section. Additional information about the separate setups will be given where needed.

3.2.1 The Mixedness Criterion

In both production processes and laboratory experiments a criterion is needed to determine whether a blending process has been successfully completed. The mixing requirements depend on the type of process or product. When liquids are blended in order to react chemically, very intense and rapid mixing is called for, especially when the kinetics of the reactions are fast. When, on the other hand, liquids are blended to change physical properties like viscosity or colour, the demands are much lower. In the paint industries, for example, there is strictly speaking no need to blend on a scale much smaller than that of the size of the tin used for further distribution of the paint, the only requirement being that all tins must contain the same amount of all components.

In the literature about mixing time measurements the most commonly used criterion is based on the disturbance in a physical quantity. A possible way of creating this disturbance is the injection of a hot or saline liquid. After the injection, the physical quantity—in the examples the temperature and the conductivity, respectively—is measured in a region of the vessel as a function of time. The most frequently applied techniques employ changes in temperature, conductivity, colour or pH, values of which are measured in a single point or integrated over a line in the vessel.

In the present work a conductivity method was used. The period after which the deviations from the final value remain within a fraction $\Delta$ of the total conductivity step is termed the mixing time. The choice of the criterion $\Delta$ strongly influences the measured mixing time. Two extreme situations are clear: if $\Delta=1$, homogeneity is instantaneous; if $\Delta=0$, homogeneity will never be achieved. The dependence of the mixing time on the criterion between these extremes is not clear. Hoogendoorn & Den Hartog (1967) propose a formula for comparing measurements carried out with differing criteria:

$$\frac{t_1}{t_2} = \frac{\ln(\Delta_1)}{\ln(\Delta_2)},$$

(3.1)

where $\Delta_1$ and $\Delta_2$ are values used for $\Delta$, and $t_1$ and $t_2$ the corresponding mixing times. When applied to actual data, even to those supplied by Hoogendoorn & Den Hartog themselves, however, this approach overestimates the differences in $t_m$, probably because the measured response curves deviate from the supposed correlation.
In the measurements reported here, a value of 0.05 for \( \Delta \) was used throughout. This value for the criterion is most often used in the literature on mixing time measurements with conductivity probes, where this criterion is often called the 95% criterion. However, as the criterion is applied to deviations on either side of the final concentration (i.e. 105% as well as 95%), a notation that includes the deviation is to be preferred.

In the course of the project the conductivity measurements were gradually computerised. The first measurements were carried out using an x-t-recorder and the acquired data were analysed by hand afterwards. The mixing time was found by checking the measured curves backwards and determining the time after which the conductivity does not exceed the criterion. Later, the data were collected by computer and stored on disc. A Pascal program analysed the data. The differences between the times found manually and those calculated by the program were small compared with the standard deviation in the repeated measurements.

Both methods have their own characteristics. In the manual method, the experimenter interprets the curve's signal to noise ratio, its general trend, possible outliers, etc. It is very difficult to incorporate these tests in a computer program reliably. Therefore, it has proved to be valuable to check the curves even when they are analysed automatically.

3.2.2 The Conductivity Probe

A matter closely related to the mixedness criterion is that of probe size. Here, as in the case of the criterion, two limit cases are clear: a probe as large as the vessel will immediately give the final concentration; a hypothetical probe with molecular dimensions will never give a constant signal because each molecule entering the probe volume will result in a large relative change in signal. The information in the literature on the effect of probe size between these two extremes is limited and contradictory. Thyên & al. (1976) show measurements with a wide variety of probe volume to vessel volume ratios. Their measurements suggest there is a decrease in measured mixing time when the probe volume is increased. Rielly & Britter (1985), on the other hand, find only a very small decrease. However, they assume the probe size to be proportional to the length of the electrode. The resulting volume is most unlikely to be representative of the actual probe volume. Our measurements in the 29 cm vessel seem to confirm the findings of Thyên & al. that the probe volume does affect the measured mixing times. Decreasing the probe volume from 160 to 60 mm\(^3\) causes an increase of 12% in the mixing time, which is smaller than the standard deviation. This effect was not extensively examined. For the results on one scale, there are no problems as long as the same probe size is used throughout. For scale-up, the matter is more complicated and neither the literature, nor our own results yield clear conclusions here.
For the present work, probes similar to those developed by Khang & Fitzgerald (1975) were used (see figure 3.1). Since the probes were handmade their dimensions were not exactly the same for all measurements. The outer electrode, which is earthed, shields the inner one from stray fields. The volume enclosed by the outer electrode is about 160 mm$^3$.

Several probe positions were tested: behind a baffle, in the stirrer discharge stream and in the centre of the circulation loop that is formed by the flow in the vessel. The only significant difference between the measured mixing times occurred in the transition region between turbulent and laminar flow: for $Re = 200$ in the 29 cm vessel, $N\cdot t_m$ is three times higher behind a baffle than in the stirrer stream (see section 3.4.1).

### 3.2.3 Vessels & Stirrers

In the literature on turbulent mixing no real standard geometry for experimental equipment has ever been agreed upon. Usually the vessels are cylindrical and fitted with four baffles. The liquid height $H$ almost invariably equals the vessel diameter $T$, and the stirrer, if there is only one, is mounted at a distance $C$ equal to its diameter $D$ from the bottom. The ratio of stirrer to vessel diameter, however, varies between 0.25 and 0.45, although values of 0.1 and 0.54 are also found.

The mixing time measurements for the present study have been carried out in geometrically identical perspex vessels of two sizes, 29 cm and 64 cm diameter. The geometry of the vessels is shown in figure 3.2. The vessels were fitted with four baffles. There was no gap between the baffles and the vessel wall.
The vessels were mounted with several types of stirrer (see figure 3.3): six-bladed disc turbines (denoted henceforth by DT), downward pumping 45° pitched 6-blade turbines (PBT) and, only in the 64 cm vessel, a Lightnin A310 mixer. The main dimensions of the stirrers are given in table 3.1. The blade width is 0.2\,D, except for that of the A310, which varies over the blade.

Figure 3.3. Impellers used for the mixing time measurements. 
Top left: disk turbine; bottom left: pitched blade turbine; right: Lightnin A310.
Drawings by A. Schinkel.
Table 3.1. Stirrer dimensions: \( T \): vessel diameter; \( D \): stirrer diameter; \( L \): blade length; \( T_b \): blade thickness; \( D_D \): central disc diameter.

<table>
<thead>
<tr>
<th></th>
<th>( T ) (cm)</th>
<th>( D ) (mm)</th>
<th>( L ) (mm)</th>
<th>( T_b ) (mm)</th>
<th>( D_D ) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DT</td>
<td>29</td>
<td>116</td>
<td>29</td>
<td>2</td>
<td>218</td>
</tr>
<tr>
<td>PBT</td>
<td>29</td>
<td>116</td>
<td>45</td>
<td>2</td>
<td>27</td>
</tr>
<tr>
<td>PBT</td>
<td>64</td>
<td>254</td>
<td>98</td>
<td>4</td>
<td>59</td>
</tr>
<tr>
<td>A310</td>
<td>64</td>
<td>254</td>
<td>100</td>
<td>var.</td>
<td>45</td>
</tr>
</tbody>
</table>

Figure 3.4. Combination of pipette and conical tube used for injection.

Additions were made in three ways:
- using a pressure vessel and a capillary tube;
- using a pipette with a wide mouth;
- using a pipette with a wide mouth and a plastic conical tube (see figure 3.4).

The last method was used in order to get reproducible, almost spherical drops, by screening the forming drops from the flow. The behaviour of spherical drops is more easily simulated than that of randomly deformed drops. The main disadvantage of introducing the conical tube into the vessel is the possible disturbance of the flow field. This turned out to be of minor influence.

The position of the injection was also varied: near the impeller, at the surface or in the bulk. The volume of liquid added was always very small compared with that of the bulk liquid: the volume ratio \( V_a/V \) was typically of order \( 10^{-5} \) to \( 10^{-4} \). Rielly & Britter (1985) found no significant effect of changing \( V_a \) in the range of 5 to 120 cm\(^3\) in a 29 cm vessel. In most of the experiments in the present work the added volume size was 3 cm\(^3\) in the 29 cm (19 dm\(^3\)) vessel and 5 cm\(^3\) in the 64 cm (206 dm\(^3\)) vessel.

3.2.4 Liquids

The liquids used in all experiments were water based, so all liquids were mutually miscible. In most of the experiments poly-vinyl-pyrrolidone (PVP) was dissolved in the water. PVP raises the viscosity as well as the density of the solvent. In a small number of experiments sodium carboxymethyl cellulose (CMC) was used to raise the viscosity. In some cases sugar syrup and glycerol were used to raise both the viscosity and the
density. Ethanol and NaCl were used to change the density. In order to raise the conductivity of the addition, NaCl and NaOH were used. In total, densities ranged from 900 to 1500 kg/m³. The density difference $\Delta \rho$, defined here as the density of the added liquid, $\rho_a$, minus the density of the bulk liquid, $\rho_0$, ranged from $-100$ to $+400$ kg/m³. Viscosities ($\mu$) ranged from 1 to $10^4$ mPa·s. For reference, table 3.2 lists the combinations of liquids used in the experiments.

The liquids containing CMC or PVP are non-Newtonian. CMC was only used in a small number of experiments that did not show any differences caused by viscoelasticity. The PVP solutions were slightly shear thinning. However, the power law index always exceeded 0.9, which is close enough to 1 to assume the liquid to be Newtonian.

Because the liquids are miscible there is no interfacial tension, so the added liquid does not form a sphere. Nevertheless, in this thesis, as in the literature on miscible liquids, the word *drop* is used to indicate parts of the added liquid.

### Table 3.2. Overview of fluids used in the experiments.

<table>
<thead>
<tr>
<th>section</th>
<th>$T$ cm</th>
<th>$\mu$ bulk mPa·s</th>
<th>$\mu$ addition mPa·s</th>
<th>$\Delta \rho$ kg/m³</th>
<th>figures</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.3 visualisation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.3.1 near stirrer</td>
<td>29</td>
<td>24 P</td>
<td>1...350 P</td>
<td>varied</td>
<td>5 through 10</td>
</tr>
<tr>
<td></td>
<td>29</td>
<td>1...115 P</td>
<td>1...100 †</td>
<td>&lt;0</td>
<td>12, 13</td>
</tr>
<tr>
<td>3.4.2 in bulk</td>
<td>29</td>
<td>9 P</td>
<td>1...100 †</td>
<td>−100...0</td>
<td>table 3</td>
</tr>
<tr>
<td></td>
<td>29</td>
<td>10 †</td>
<td>2...1000 †</td>
<td>−100...−5</td>
<td>14, 16, 17, 18</td>
</tr>
<tr>
<td></td>
<td>64</td>
<td>1</td>
<td>5...100 †</td>
<td>−50...−5</td>
<td>19, 20</td>
</tr>
<tr>
<td></td>
<td>64</td>
<td>8 P</td>
<td>58 †</td>
<td>−100...−5</td>
<td>21</td>
</tr>
<tr>
<td></td>
<td>64</td>
<td>1</td>
<td>5...100 †</td>
<td>−70</td>
<td>22</td>
</tr>
<tr>
<td>3.4.3 at surface</td>
<td>29</td>
<td>9 †</td>
<td>≈13 †</td>
<td>−70</td>
<td>23</td>
</tr>
<tr>
<td></td>
<td>64</td>
<td>1...8 P</td>
<td>86...1500 †</td>
<td>≈−20</td>
<td>table 4</td>
</tr>
<tr>
<td></td>
<td>64</td>
<td>1</td>
<td>54...360 †</td>
<td>−80...−70</td>
<td>24</td>
</tr>
<tr>
<td>3.5.1 near stirrer</td>
<td>29</td>
<td>1</td>
<td>1...1470 C, P, S</td>
<td>&gt;0</td>
<td>table 5</td>
</tr>
<tr>
<td>3.5.2 in bulk</td>
<td>29</td>
<td>1</td>
<td>2800 S</td>
<td>380</td>
<td>25</td>
</tr>
<tr>
<td>or at surface</td>
<td>29</td>
<td>1...10 †</td>
<td>125...5000 †</td>
<td>&gt;0</td>
<td>table 6</td>
</tr>
<tr>
<td></td>
<td>64</td>
<td>1</td>
<td>4700 S</td>
<td>400</td>
<td>26</td>
</tr>
<tr>
<td></td>
<td>64</td>
<td>1</td>
<td>4700 S</td>
<td>400</td>
<td>27, 28</td>
</tr>
</tbody>
</table>

C water & CMC
P water & PVP
S water & sugar syrup
† water & ethanol/glycerol/PVP
3.2.5 Repeat Measurements

For each condition five to twenty measurements were carried out consecutively, giving average values for $N_f_m$. The number of repeat measurements depended on the scatter in the results and on the type of liquid: some liquids, especially the high viscosity additions, have a very long preparation time; furthermore, with high viscosity additions the bulk is rapidly contaminated by the addition, preventing further experiments.

In those cases where only a limited number of experiments could be done, a larger number of experimental conditions was chosen rather than more experiments per condition. This results in a smaller significance for each experimental condition, but trends can be seen more readily. As a rule of thumb, differences that are larger than the standard deviation within a series of measurements, $\sigma$, will be regarded significant.

It should be emphasised here that the average of $N_f_m$ was calculated by determining the mixing time for each individual measurement and averaging those values, and not by averaging the conductivity responses and determining a mixing time from the averaged curve. The mixing times arrived at by the last method are too short because the averaged curves are too smooth.

3.3 Visualisation

Photographs were taken to get a better idea of the mechanisms that cause homogenisation$^1$. The photographs show the 29 cm vessel filled with water containing PVP, stirred by a PBT. The bulk viscosity, $\mu_0$, was about 24 mPa·s, the stirrer rotational speed 2 s$^{-1}$, so $Re \approx 1200$. Coloured liquid was added using a 5 mm inner diameter pipette, so that the liquid entered the bulk as an elongated drop. In this setup the stirrer pumps downwards, so the stirrer blades closest to the viewer as well as the liquid in front move to the right. The grey vertical band that is visible under the impeller is the baffle on the far side of the vessel. The baffle in front has been removed to allow an unobstructed view.

The first photograph, figure 3.5, shows the addition of water, $\mu_a = 1$ mPa·s, about 0.2 s after first contact with the stirrer. The thin stream of liquid flowing from the pipette is a small leak flow following the main addition. Figure 3.6 shows the same process, 0.5 s later. The shearing of the added liquid by the bulk causes diffuse sheets.

Figures 3.7 and 3.8 are photographs that were made with a 350 mPa·s addition, at the same time intervals. The liquid is deformed into diffuse threads rather than into sheets.

The threads are even more pronounced in figures 3.9 and 3.10, where $\mu_a \approx 1600$ mPa·s. These photographs were also taken about 0.2 and 0.7 s after first contact with the stirrer. The liquid forms a long continuous line that is constantly being deformed by the turbulent motions.

The photographs show that low viscosity additions are deformed into sheets, whereas high viscosity additions form threads. This is sketched schematically in figure 3.11. The existence of two deformation mechanisms hampers the modelling, because the rate at which the addition gets thinner is different in each case.

$^1$All photographs by A. Schinkel.
Figure 3.5. Photograph of mixing process, taken about 0.2 s after first contact with stirrer; $\mu_0 = 24 \text{ mPa\cdot s}$, $\mu_a = 1 \text{ mPa\cdot s}$; $N = 2 \text{ s}^{-1}$.

Figure 3.6. Photograph taken 0.5 s after the previous photograph.

Figure 3.7. Photograph of mixing process, taken about 0.2 s after first contact with stirrer; $\mu_0 = 24 \text{ mPa\cdot s}$, $\mu_a = 350 \text{ mPa\cdot s}$; $N = 2 \text{ s}^{-1}$.

Figure 3.8. Photograph taken 0.5 s after the previous photograph.
A closer examination of the last two photographs gives information about the rate of deformation of the added high viscosity liquid. The liquid was added as an elongated cylindrical drop of about 3 cm length and 1 cm diameter.

The most important dimension of the deforming cylindrical drop in view of diffusion is its diameter, perpendicular to its long axis. This diameter decreases as a function of time, as can be seen from the thickest part of the thread in figures 3.9 and 3.10. In the 0.5 s period between the photographs the diameter of this part is about halved. Moreover, the diameter of all parts of the deformed drop appears to have been reduced to about half its value in that period. At this rate the thickness of the added drop would be reduced to one thousandth of its initial value within 5 s. The photographs show that the threads moved in a region with neither extremely high shear rates nor shear free conditions. The reduction in thickness may therefore be taken as an estimate for the average over the vessel.
The fast decrease of the smallest dimensions of the added liquid, even at high viscosity ratios, shows that the added liquid viscosity is not the main factor determining the homogenisation time. This will be analysed further in the next chapter.

3.4 Mixing Time Measurements with $\Delta \rho < 0$

The density difference $\Delta \rho$ is defined here as the density of the added liquid, $\rho_a$, minus the density of the bulk liquid, $\rho_0$. Therefore, for buoyant additions $\Delta \rho < 0$. This situation will be treated first.

3.4.1 Addition near the Stirrer

When buoyant liquid is added near the stirrer, the upward forces are not strong enough to transport the addition to the surface. Moreover, in the vicinity of the stirrer the shear stresses and turbulence intensities are high, so that the added liquid is rapidly distorted, which further reduces buoyancy effects. This will be referred to as stirrer controlled mixing.

Figure 3.12 shows the results of experiments with a PBT for a probe positioned in the stirrer plane. The additive was tap water with salt added for the purpose of the conductivity measurements. Data processing was done by hand. The standard deviation within the series of ten measurements varies, not systematically, between 10 and 20%. For bulk viscosities up to 115 mPa·s the dimensionless mixing times are constant in the turbulent regime. For $Re$ lower than 1000, i.e. in the turbulent to laminar transition regime, the

![Graph showing $N\cdot t_m$ vs. Re for probe in stirrer plane.](image)
mixing times are higher. Figure 3.13 shows the results of the same series of measurements for a second probe, positioned close to the bottom of the vessel behind a baffle. In the turbulent regime the mixing times are about the same as for the first probe, but in the transition region $N\cdot t_m$ can be 3 times higher behind the baffle. These longer mixing times dominate the blending process, so clearly the transition region should be avoided.

In later experiments the viscosities and densities of both bulk and addition were varied independently. Typical examples of dimensionless mixing times are given in table 3.3 for $\mu_0 \approx 10$ mPa·s, all in the turbulent regime. The viscosity ratio $\mu_a/\mu_0$ is denoted by $\mu^*$. The average value of $N\cdot t_m$ for the table is 26. The standard deviation within each series of six measurements, $\sigma$, varies, not systematically, between 11 and 19%. The difference between the lowest value and the highest value in the table is 6, which is only a little more than $\sigma$, so again the correlation of $N\cdot t_m = \text{constant}$ can be used.

**Table 3.3. Dimensionless mixing times for various viscosity ratios and density differences; $Re = 1.6 \cdot 10^3$ in all cases.**

($T = 29$ cm; $\mu_0 \approx 10$ mPa·s; PBT; addition near the stirrer)

<table>
<thead>
<tr>
<th>$\Delta \rho$ (kg/m$^3$)</th>
<th>0.1</th>
<th>1.0...1.8</th>
<th>10...14</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>25</td>
<td>26</td>
<td>29</td>
</tr>
<tr>
<td>-20</td>
<td>24</td>
<td>28</td>
<td>27</td>
</tr>
<tr>
<td>-100</td>
<td>30</td>
<td>25</td>
<td>24</td>
</tr>
</tbody>
</table>
3.4.2 Addition in the Bulk

*Three Regimes*

Addition of the liquid at positions far from the stirrer result in different mixing mechanisms. Experiments with a PBT in the 29 cm vessel, partly reported on by Bouwmans & Van den Akker (1990), showed that the mixing time is strongly influenced by viscosity and density differences when 3 cm³ of a tracer liquid is injected about 1 cm below the free surface. Figure 3.14 shows the dimensionless mixing times versus Re in this situation for six combinations of liquids: \( \mu_0 = 10 \text{ mPa} \cdot \text{s} \).

For \( \Delta \rho = -5 \text{ kg/m}^3 \) and \( \mu^* = 0.11 \) (open squares) the mixing time corresponds to that of addition near the stirrer. The value of \( N \cdot t_m \) is about 30 for \( Re > 10^3 \). For the whole range of \( Re \) the stirrer frequency is high enough to produce a strong large-scale flow that can overcome buoyancy forces so that the added liquid is transported to the stirrer region, where the drop is broken up. This will be called the *stirrer controlled regime*, by analogy with the case of addition near the stirrer (previous section). Figure 3.15 (a) shows a possible resulting conductivity response. The probe registers the first two or three passages of saline liquid, but each passage the passing becomes less pronounced. In this example, \( N \cdot t_m \approx 25 \). For \( Re \approx 10^3 \) the mixing time is more than 30% higher than 30 (see figure 3.14). This is more than the standard deviation, \( \sigma \), and the increase is caused by the turbulent to laminar transition, as in figure 3.12. All other open squares lie in the turbulent regime: \( Re \) is larger than \( 10^3 \).

![Figure 3.14. \( N \cdot t_m \) versus Re for six combinations of liquids. The dotted lines are intended to guide the eye.](image)

\((T = 29 \text{ cm}; \mu_0 = 9 \text{ mPa} \cdot \text{s}; V_a = 3 \text{ cm}^3; \text{PBT; addition in bulk})\)
In the other two cases with $\mu^* = 0.11$ (open diamonds & open triangles) the buoyancy forces are stronger than the forces exerted on the added liquid by the bulk flow, so all or part of the additive rises to the surface. The liquid is then slowly merged with the bulk by turbulent eddies, which results in mixing times that can be ten times longer than in the stirrer controlled regime. The regime where all of the added liquid rises to the surface will be termed the gravity controlled regime. In this regime the conductivity curve is much smoother (see figure 3.15 (c), where $N \cdot t_m \approx 150$): the breakdown of the layer at the surface by the turbulent eddies is a continuous process. The regime between the stirrer controlled regime and the gravity controlled regime will be called the intermediate regime. The conductivity response in this case is a combination of the other curves, as can be seen in figure 3.15 (b) (where $N \cdot t_m \approx 80$). Sharp peaks during the first seconds indicate the passage of liquid that has been pulled down into the stirrer. The smooth second part of the curve is caused by the mixing of the remaining fluid from the surface.

Figure 3.14 also shows the effect of $\mu^*$ on $N \cdot t_m$ for a constant density difference. For $\Delta \rho = -5 \text{ kg/m}^3$ (squares) the dimensionless mixing time is higher for $\mu^* = 10$ (solid squares) than for $\mu^* = 0.11$ (open squares). When the viscosity of the added liquid is high, the addition is less deformed by the mean flow. Less deformed drops experience smaller friction forces from the mean flow, resulting in larger upward velocities. In that case the liquid is more likely to reach the surface, which would result in the intermediate or gravity controlled regime.

For more negative values of $\Delta \rho$ (diamonds & triangles) the mixing time is also affected by $\mu^*$: higher values of $\mu^*$ (solid markers) result in longer mixing times, because larger portions of the added liquid reach the surface. Moreover, once the addition has reached the surface, higher viscosities more strongly resist mixing by the bulk.
The Richardson Number

From figure 3.14 it is clear that the three mixing regimes cannot be distinguished on the basis of $Re$. A dimensionless group that does include the density difference is the Richardson number (see for instance Rielly & Pandit (1988)):

$$Ri = \frac{\Delta \rho g H}{\rho_0 N^2 D^2} \quad (3.2 = 2.10)$$

(with $g$ the gravitational acceleration and $H$ the liquid height in the vessel). It is a measure for the ratio of the potential energy needed to transport the added liquid to the stirrer and the kinetic energy of the bulk. The dimensionless mixing time as a function of the absolute value of $Ri$ is given in figure 3.16 for the same measurements as in figure 3.14. The figure shows that $Ri$ sorts the data better than $Re$ does, because buoyancy effects are taken into account. However, the viscosity ratio is not included in $Ri$, and two bands can be seen, one for $\mu^* = 0.11$ (open markers) and one for $\mu^* = 10$ (solid markers).

Figure 3.17 shows the same data. The stirrer controlled regime and the gravity controlled regime—both determined by visualisation—are indicated by shading. The boundaries of the regimes are not sharp. Two data points have been added: one for $\mu_0 = 1$ mPa·s (solid circle) and one for $\mu_0 = 40$ mPa·s (open circle). The regime they belong to is the same as that of the neighbouring data points. However, they fall outside the band of data and the mixing time for the solid circle is almost that of the stirrer controlled regime. This shows that the bulk viscosity is an essential factor in the eventual gravity controlled mixing time.

**Figure 3.16. $N\cdot t_m$ versus the absolute value of $Ri$ for six combinations of liquids.**

The dotted lines are intended to guide the eye.

($T = 29$ cm; $\mu_0 = 9$ mPa·s; $V_a = 3$ cm$^3$; PBT; addition in bulk)
Figure 3.17. The measurements of 3.16 and two extra data points; regimes are indicated by shading; \( \mu_0 = 9 \text{ mPa s} \), except in those cases indicated by circles.

\( T = 29 \text{ cm}; \mu_0 = 9 \text{ mPa s}; V_a = 3 \text{ cm}^3; \text{PBT; addition in bulk} \)

Figure 3.18. The relative standard deviation within the measurement series against \( |R_i| \). \( T = 29 \text{ cm}; \mu_0 = 9 \text{ mPa s}; V_a = 3 \text{ cm}^3; \text{PBT; addition in bulk} \)

In the intermediate region, where only part of the added liquid rises to the surface, the standard deviation within a series of repeat measurements is high. Figure 3.18 gives the relative standard deviation \( \sigma(t_m)/t_m \) as a function of \( |R_i| \). For \( 0.2 < |R_i| < 4 \) the standard deviation reaches values of up to 80%, whereas outside that region the deviation remains below 30%.
The unpredictability of the mixing time in the intermediate regime is caused by the unpredictability of turbulent motion. In this regime the forces exerted on the addition by the bulk flow are of the same order as the buoyancy forces. Therefore, the turbulent part of the local velocity at the moment of addition determines the fate of the injected liquid. Moreover, the liquid contained in one drop does not always follow one path: very often part of the drop rises to the surface while the rest of the drop is transported to the stirrer where it is broken up. The amount of liquid that reaches the surface determines the mixing time, as will be shown in the next section. Due to this effect, the resulting mixing times can have any value from the stirrer controlled mixing time on the low side to the gravity controlled mixing time on the high side. This results in a large standard deviation in the mixing times.

• *The Combined Effect of Density and Viscosity Differences*

A characteristic of the $N_t \cdot \tau_m$ vs. $|Ri|$ graphs is the bend between the stirrer controlled regime and the intermediate regime. Above this bend the mixing times depend on the amount of liquid rising to the surface, whereas for lower values of $|Ri|$ the mixing time is constant. As may be expected from the results discussed earlier, the location of the bend depends on the properties of the liquids being blended.

In figure 3.19 the stirrer rotational speed where this transition occurs, $N_1$, is given as a function of the density difference and the viscosity of the added liquid. The value of $N_1$ proved to be independent of the criterion that is used to define the mixing time. The experiments were carried out with the conical tube described in section 3.2.2. The bulk viscosity is about 10 mPa·s. Drops were added 10 cm below the surface at a radial distance of 10 cm, 5° behind a baffle.

**Figure 3.19.** Stirrer rotational speed (s⁻¹) at the transition between the intermediate regime and the stirrer controlled regime, as a function of $\mu_a$ and $\Delta \rho$.

*The dotted lines are intended to guide the eye.*

($T = 29$ cm; $\mu_0 \approx 10$ mPa·s; $V_a = 3$ cm³; PBT; addition in bulk)
Chapter Three

![Graph](image)

**Figure 3.20. Enlarged detail of figure 3.19 for high viscosity additions.**

The dotted lines are intended to guide the eye.

\(T = 29\,\text{cm}; \mu_0 = 10\,\text{mPa}\cdot\text{s}; V_a = 3\,\text{cm}^3; \text{PBT; addition in bulk}\)

The figure shows that for \(\mu_a < 100\) the value of \(N_t\) depends on \(\mu_a\) as well as on \(\Delta\rho\). For higher values of \(\mu_a\) the dependence is much lower (see figure 3.20): above a given value of \(\mu^*\) the deformation after injection is so low that a further increase in \(\mu_a\) does not change the chance of surfacing.

With buoyant additions of very high viscosity \((\mu_a \geq 10\,\text{Pa}\cdot\text{s})\), mixing can be even less predictable than for lower added liquid viscosities, for then there are more than two possibilities.

- When the liquid rises to the surface it may remain there while it is slowly blended into the bulk. It may also form a long thread extending from the surface to the stirrer where it is mixed. Eventually, the thread is totally pulled down into the stirrer and mixed.

- The addition may also go to the stirrer. In that case the mixing is fast and usually \(N_t\) does not significantly differ from 30.

- When the liquid goes neither to the surface nor to the stirrer, it floats in the bulk liquid, the buoyancy forces about equaling the downward forces exerted by the mean flow. The shear forces and pressure forces in the bulk may then be too weak to blend the high viscosity liquid quickly. Longer mixing times will result in this case. When by chance the addition is transported to the stirrer the mixing will be fast from then on.

**Addition in the Bulk in the 64 cm Vessel**

In the stirrer controlled regime, dimensionless mixing times in the 64 cm vessel are about equal to those in the 29 cm vessel. Characteristic stirrer controlled mixing times for the larger vessel are given in figure 3.21. In these experiments the stirrer speed was 2 s\(^{-1}\), and 5 cm\(^3\) of a saline liquid was injected 3 cm below the liquid surface near the
Figure 3.21. $N\cdot t_m$ as a function of $\mu_a$ and $\Delta \rho$ for the PBT.

$(T = 64 \text{ cm}; \mu_0 = 1 \text{ mPa s}; V_a = 5 \text{ cm}^3; \text{PBT; addition in bulk})$

shaft. The bulk was tap water. The figure shows there is no systematic influence of either $\mu_a$ or $\Delta \rho$ on the dimensionless mixing time. The standard deviations are low, ranging from 10% to 23%, again not systematically.

Mixing times were also measured with PVP dissolved in the bulk: $\mu_0 = 8 \text{ mPa s}$ and $\rho_0 = 1003 \text{ kg m}^{-3}$. The stirrer speed was 3 s$^{-1}$. The added liquid properties were $\mu_a = 60 \text{ mPa s}$ and $\rho_a = 933 \text{ kg m}^{-3}$, so $\Delta \rho = -70 \text{ kg m}^{-3}$. The added liquid volume was 5 cm$^3$, injected as a cylinder with a diameter of about 6 mm. The dimensionless mixing times are given at three positions in figure 3.22. The positions were between the shaft and a baffle, 5 cm below the liquid surface at radial distances of 0.2, 0.4 and 0.6 times the vessel radius. Here, again, $N\cdot t_m$ is low. The corresponding relative standard deviations, given in the same figure, are low as well.

Figure 3.22. $N\cdot t_m$ at three injection positions.

Relative standard deviations are also given below the mixing times.

$(T = 64 \text{ cm}; \mu_0 = 8 \text{ mPa s}; \mu_a = 60 \text{ mPa s}; \Delta \rho = -70 \text{ kg m}^{-3}; V_a = 5 \text{ cm}^3; \text{PBT})$
These mixing times seem to suggest stirrer controlled mixing. However, visual observation showed that at the middle position the mixing is in the intermediate regime, while at the position closest to the baffle the mixing is gravity controlled. Later tests with addition at the surface revealed that the low mixing times were caused by the fact that the volume of added liquid for figure 3.22 was only small. As will be shown in the section on addition at the surface, the mixing time increases for larger added liquid volumes.

The mixing times in the stirrer controlled regime (figures 3.21 and 3.22, left) are longer than those in the gravity controlled regime (figure 3.22, right), but the difference is about equal to the standard deviation $\sigma$. Because there is no significant difference between the stirrer controlled mixing time and the gravity controlled mixing time for $V_a = 5 \text{ cm}^3$, the standard deviation for the middle position in 3.22 is not higher than that of the other two positions, contrary to the situation in the 29 cm vessel.

**Addition in the Bulk Using the A310**

An A310 stirrer was also tested in the 64 cm vessel under the same conditions as for figure 3.21 ($N = 2 \text{ s}^{-1}$; $5 \text{ cm}^3$ injected 3 cm below surface; water as bulk). Visualisation showed that the mixing was stirrer controlled in all cases. The values of $N \cdot t_m$ are about 1.8 times those of the PBT, as can be seen in figure 3.23. The standard deviation ranges from 16% to 23%.

![Graph](image)

*Figure 3.23. $N \cdot t_m$ as a function of $\mu_a$ and $\Delta \rho$ for the A310.*

(T = 64 cm; $\mu_0 = 1 \text{ mPa} \cdot \text{s}$; $V_a = 5 \text{ cm}^3$; A310; addition in bulk)

The energy needed for homogenisation is equal to

$$E_m = P \cdot t_m = P_0 \rho_0 N^3 D^5 t_m .$$

(3.3 = 2.3)

The values of $P_0$ in the turbulent regime for the PBT and the A310 were measured using
a torque meter and were 1.44 and 0.29, respectively. For equal stirrer rotational speeds, formula 3.3 results in:

\[
\frac{E_{m, A310}}{E_{m, PBT}} = \frac{P_0 A310 (N t_m) A310}{P_0 PBT (N t_m) PBT} \approx 0.36 ,
\]

which means that, although it takes longer to achieve homogeneity with the A310, the consumed energy is much less: in this case 65 J for the A310 and 182 J for the PBT. However, in order to achieve the same mixing time as with the PBT, the A310 should be operated at a higher stirrer rotational speed. For equal mixing times, formula 3.3 yields:

\[
\frac{E_{m, A310}}{E_{m, PBT}} t_m = \frac{P_0 A310 (N t_m)^3 A310}{P_0 PBT (N t_m)^3 PBT} \approx 1.17 .
\]

This means that more energy is required for blending with the A310 (213 J) than is needed with the PBT. It can be concluded that for the given geometry the A310 is more efficient if a short mixing time is not the first requirement, but the PBT is preferred when the mixing time is fixed.

For equal power input, the ratio of the required energies is

\[
\frac{E_{m, A310}}{E_{m, PBT}} = \frac{t_m A310}{t_m PBT} = \frac{(N t_m) A310}{(N t_m) PBT} \frac{N_{PBT}}{N_{A310}} ,
\]

which, using

\[
N = \left[ \frac{P}{P_0 \rho D^3} \right]^{1/3} ,
\]

gives

\[
\frac{E_{m, A310}}{E_{m, PBT}} = \frac{(N t_m P_0^{1/3}) A310}{(N t_m P_0^{1/3}) PBT} = \left[ \frac{E_{m, A310}}{E_{m, PBT}} \right]^{1/3} \approx 1.05 .
\]

Therefore, at equal power draw the energies required for homogenisation are equal within the experimental deviations.

It is also possible to use an A310 that is about 20% larger. This yields the same mixing times as the PBT, while both the power input and the torque are lower (Weetman (1992)). Lower torque reduces the initial costs of the equipment. As it was beyond the scope of this project, however, the effect of changing the stirrer diameter was not analysed further.

3.4.3 Addition at the Surface

For some series of measurements liquid was deliberately added at the surface. As will be shown here, in those cases the mixing time depends on the amount of liquid added.

For the 29 cm vessel, addition at the surface was done with \( \mu_0 = 9 \text{ mPa:s} \). The result is given in table 3.4. The dimensionless mixing time increases as more liquid is added.
Table 3.4. $N\cdot t_m$ for surface addition in 29 cm vessel.

\[ (T = 29 \text{ cm}; \mu_0 = 9 \text{ mPa} \cdot \text{s}; \text{PBT}) \]

<table>
<thead>
<tr>
<th>$V_a$ cm$^3$</th>
<th>$\Delta \rho$ kg/m$^3$</th>
<th>$\mu^*$</th>
<th>$N$ s$^{-1}$</th>
<th>$N\cdot t_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>-18</td>
<td>1.6</td>
<td>1.45</td>
<td>114</td>
</tr>
<tr>
<td>30</td>
<td>-22</td>
<td>1.3</td>
<td>1.75</td>
<td>164</td>
</tr>
</tbody>
</table>

The results for an addition of 20 cm$^3$ in the 64 cm vessel are shown in figure 3.24. The circles are data for a bulk of 8 mPa·s. The mixing times increase with increasing $|\text{Re}|$, which corresponds to decreasing $N$. For $|\text{Re}| = 6$ ($N = 1 \text{ s}^{-1}$) the dimensionless mixing time is also given for a bulk of 1 mPa·s (squares). These times are all much shorter than those for the more viscous bulk, even though the viscosities of the added liquids are much higher. The viscosity of the bulk plays a crucial part in this type of mixing. The reason is the difference in size of the turbulent eddies: less viscous liquids have a larger range of eddy sizes, as indicated by Kolmogorov’s length scale.

Figure 3.24. Dimensionless mixing times versus $|\text{Re}|$

\[ (T = 64 \text{ cm}; \Delta \rho = -70 \text{ to } -80 \text{ kg/m}^3; V_a = 20 \text{ cm}^3; \text{PBT}; \text{surface addition}). \]

Table 3.5. The effect of added liquid volume on $N\cdot t_m$; $N = 0.5 \text{ s}^{-1}$; $V_a = 5 \text{ ml}$; $V_a = 20 \text{ ml}$

<table>
<thead>
<tr>
<th>$\Delta \rho$ kg/m$^3$</th>
<th>$\mu^*$</th>
<th>$N\cdot t_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBT</td>
<td>-81</td>
<td>54</td>
</tr>
<tr>
<td>PBT</td>
<td>-68</td>
<td>360</td>
</tr>
<tr>
<td>A310</td>
<td>-85</td>
<td>58</td>
</tr>
<tr>
<td>$V_a = 5 \text{ ml}$</td>
<td></td>
<td>34</td>
</tr>
<tr>
<td>$V_a = 20 \text{ ml}$</td>
<td></td>
<td>40</td>
</tr>
<tr>
<td></td>
<td></td>
<td>46</td>
</tr>
<tr>
<td></td>
<td></td>
<td>64</td>
</tr>
<tr>
<td></td>
<td></td>
<td>57</td>
</tr>
<tr>
<td></td>
<td></td>
<td>67</td>
</tr>
</tbody>
</table>
Table 3.5 shows the effect of added liquid volume on mixing times. The stirrer speed in these examples is $0.5 \text{ s}^{-1}$, $\mu_0 = 1 \text{ mPa} \cdot \text{s}$ ($Re = 3.3 \cdot 10^4$). As mentioned before, the mixing times for small amounts of added liquid equal those of the stirrer controlled regime. The Lightnin A310 mixing times are longer because of the lower power input for equal stirrer rotational speeds, as explained in the previous section. The table shows that for $\mu^* \approx 55$, $N \cdot t_m$ increases by 18%—about one standard deviation $\sigma$—when $V_a$ is quadrupled, for both the PBT and the A310. For $\mu_a = 360 \text{ mPa} \cdot \text{s}$ the increase amounts to 39%, which is more than $\sigma$. This shows that the relative increase in mixing time does not only depend on the amount of liquid added, but also on its viscosity: more viscous liquids are less easily attacked by the eddies in the bulk.

3.5 Mixing Time Measurements with $\Delta \rho > 0$

The blending of settling additions exhibits the same behaviour as that of buoyant additions. The addition may be transported to the stirrer and be deformed there. On the analogy of the buoyant case this will be called the stirrer controlled regime. The liquid may also reach the bottom of the vessel: the gravity controlled regime. As in the case of buoyant liquids this can result in very long mixing times, depending on the properties of the liquids and on the flow conditions.

3.5.1 Addition near the Stirrer

The experiments by Smith & Schoenmakers (1988) were carried out in a 29 cm vessel using a DT in a bulk of water and dilute aqueous solutions. Thick sugar syrups or solutions of CMC (1 and 2%) were used as viscous additions. The added liquid density was only controlled by the concentration of sugar syrup or CMC.

The liquid was added in the stirrer plane via a glass tube with an inner diameter of 5 mm. Immediately after the injection of the liquid, the liquid remaining in the tube was withdrawn, so that no additional liquid could flow out.

The combined results for sugar syrup additions (viscosities up to 1400 mPa·s) and CMC solution additions ($\leq 1470 \text{ mPa} \cdot \text{s}$) show that for these added liquid viscosities $N \cdot t_m$ is about 17 for $Re$ between $10^5$ and $10^6$. The power number of the DT is about three times that of the PBT. Therefore, the energies needed for homogenisation for equal $N$, $t_m$ and $P$ are (compare formulas 3.4 through 3.8):

$$\frac{E_{m, DT}}{E_{m, PBT}}_N = \frac{P_{0, DT}(N \cdot t)m_{DT}}{P_{0, PBT}(N \cdot t)m_{PBT}} \approx 1.74 , \quad (3.9)$$
\[
\begin{bmatrix}
\frac{E_{m,DT}}{E_{m,PBT}}
\end{bmatrix}_{\text{t}_{\text{m}}} = \frac{P_{0,DT}(N^3 t_m)^3_{DT}}{P_{0,PBT}(N^3 t_m)^3_{PBT}} \approx 0.56, \\
\begin{bmatrix}
\frac{E_{m,DT}}{E_{m,PBT}}
\end{bmatrix}_{\text{p}} = \frac{(N^3 t_m P_0^{1/3})_{DT}}{(N^3 t_m P_0^{1/3})_{PBT}} \approx 0.82.
\]

(3.10) (3.11)

3.5.2 Addition at the Surface or in the Bulk

Smith & Schoenmakers also measured mixing times for addition in the bulk, close to the surface in the 29 cm vessel, stirred at 3 s\(^{-1}\) by a DT. Because the additives were not only more viscous but also heavier than the bulk, the added drops (about 0.1 cm\(^3\)) tended to sink to the bottom. The percentage of drops reaching the bottom and adhering to it is given in figure 3.25, left, for five addition points. At each position 100 drops were released, so the statistical error is about ± 10.

Drops sticking to the bottom yield very long mixing times. Depending on their position they take from 1 to over 10 minutes to be dissolved, see figure 3.25, right. As \(N = 3\) s\(^{-1}\) this means dimensionless mixing times of 180 to over 1800. The danger of adhesion of the viscous material to vessel surfaces is reduced by higher impeller speeds, by introduction of the high viscosity addition in an elongated stream rather than as drops and by addition near the impeller shaft on the free surface. When care is taken to prevent the added material from sticking to fixed surfaces, the mixing time in the turbulent region is about the same as that for liquids without viscosity differences.

![Figure 3.25. Left: percentages of drops reaching the bottom; right: mixing times for drops on the bottom (after Smith & Schoenmakers). (T = 29 cm; \(\mu_0 = 1\) mPa·s; \(\mu_a = 2.8\) Pa·s; \(\Delta \rho = 400\) kg/m\(^3\); DT; surface addition)](image_url)
Smith & Schoenmakers observed that drops that do not traverse the impeller zone but remain in free suspension take about 50% longer to dissolve than those passing through the impeller zone. However, the maximum time for assimilation remained well within the measured mixing time.

In later experiments with $\Delta \rho > 0$ the viscosity and the density of both the added liquid and the bulk were varied separately. Mixtures of water, ethanol and glycerol were used, in which salt and PVP were dissolved. These experiments were carried out in a 29 cm vessel mounted with a PBT. The injection position was 2 cm below the surface. Data processing was done by computer.

The experiments show (see table 3.6) that a viscosity ratio ranging from 84 to 5000 has no influence on $N\tau_m$ for higher stirrer speeds, taking into account that the standard deviation of $N\tau_m$ is about 20%. For $\mu^*=5000$ and $Re=20\cdot10^3$ the table shows that the dimensionless mixing time increases. The increase is caused by the addition clinging to the vessel bottom or walls. This is termed the gravity controlled regime, by analogy with the case of buoyant surfacing additions. For settling liquids this regime was not examined extensively. The conclusion is that for $\mu_0 = 1$ mPa·s the dimensionless mixing time is independent of $\mu^*$ for $\mu^* < 5000$, provided the addition moves to the stirrer.

**Table 3.6. Effect of $\mu^*$ on dimensionless mixing times.**

*(T = 29 cm; $V_a=3$ cm³; PBT; $\Delta \rho \approx 60$ kg/m³; addition in the bulk)*

<table>
<thead>
<tr>
<th>$\mu_0$ (mPa·s)</th>
<th>$\mu_a$ (mPa·s)</th>
<th>$\mu^*$</th>
<th>$Re \cdot 10^3$</th>
<th>$N\tau_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>840</td>
<td>84</td>
<td>5...7</td>
<td>32</td>
</tr>
<tr>
<td>1</td>
<td>125</td>
<td>125</td>
<td>20</td>
<td>26</td>
</tr>
<tr>
<td>1</td>
<td>5000</td>
<td>5000</td>
<td>40...90</td>
<td>62</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>20</td>
<td>21...27</td>
</tr>
</tbody>
</table>

In the 64 cm vessel filled with tap water and mounted with a PBT, experiments were carried out with added drops of sugar syrup. For this combination of liquids $\Delta \rho \approx 400$ kg/m³ and $\mu^* = 4700$. The stirrer rotational speed was varied between 1.45 and 3.6 s⁻¹ ($9.4 \cdot 10^4 < Re < 2.3 \cdot 10^5$). Drops of 1 cm³ were added at the surface and sank immediately.

Figure 3.26 shows the probability of a drop reaching the bottom of the vessel as a function of addition position for $N = 2.0$ s⁻¹ (left) and 3.6 s⁻¹ (right). For each position and stirrer rotational speed 50 drops were added, which implies that the percentages have a statistical error of ±13. The chances decrease rapidly as the stirrer speed is raised, but for each stirrer rotational speed the probabilities vary less than in the experiments of Smith & Schoenmakers in the 29 cm vessel mounted with a DT.
Figure 3.26. Percentage of drops reaching the bottom for two stirrer rotational speeds. 
\(T = 64\ \text{cm}; \mu_0 = 1\ \text{mPa} \cdot \text{s}; \mu_a = 4700\ \text{mPa} \cdot \text{s}; \Delta \rho \approx 400\ \text{kg/m}^3; V_a = 1\ \text{cm}^3; \text{PBT; surface addition)}

When the drops remain on the bottom, long mixing times result, as is shown in figure 3.27 (filled circles). Larger drops (2 cm\(^3\), open circles) do not reach the bottom, and the mixing time remains about 30. This conflicts with the fact that large spheres have higher speeds relative to the surrounding liquid than small spheres have, and could be expected to reach the bottom more easily. The explanation may be that large drops may be more readily deformed and are therefore subjected to stronger convective forces by the bulk flow.

Figure 3.27. Dimensionless mixing time against Ri for two added liquid volumes. 
\(T = 64\ \text{cm}; \mu_0 = 1\ \text{mPa} \cdot \text{s}; \mu_a = 4700\ \text{mPa} \cdot \text{s}; \Delta \rho \approx 400\ \text{kg/m}^3; \text{PBT; surface addition)}

50
Figure 3.28. Times that drops remain on bottom for four sections; \( N = 1.5 \) \( \text{s}^{-1} \).  
\( T = 64 \text{ cm}; \mu_0 = 1 \text{ mPa\cdot s}; \mu_a = 4700 \text{ mPa\cdot s}; \Delta \rho = 400 \text{ kg/m}^3; V_a = 1 \text{ cm}^3; \text{PBT; surface addition} \)

As was the case in the Smith & Schoenmakers experiments (29 cm vessel, DT), the time the drops remain on the bottom depends on their position on the bottom. These times are much shorter than those found by Smith & Schoenmakers: even at a low speed of 1.5 \( \text{s}^{-1} \) the times seldom exceed 100 s. Figure 3.28 shows the distribution of times for four bottom regions. A remarkable difference from figure 3.25 is the relatively short time the drops remain behind a baffle, which must be due to a stronger baffle vortex caused by the PBT.

Another difference from the findings of Smith & Schoenmakers concerning the DT is that a drop is often removed as a whole by the stronger circulatory flow of the PBT. This makes the modelling of mixing from the bottom very complex. The liquid may remain on the bottom until it is fully blended into the bulk. Parts of the drop may be pulled upwards and mixed by the stirrer. In many cases the drop is lifted from the bottom as a whole after a short interval.

For the higher speeds \( (N \geq 2 \text{ s}^{-1}) \) the dimensionless mixing time was about 30. Almost all drops were transported to the stirrer region and deformed during one of the first passages. Some drops did reach the bottom but were scattered there. This means that in the 64 cm vessel the upper limit of the viscosity ratio with \( N\cdot t_m \approx 30 \) is at least 4500. These measurements confirm the results of the visualisation: the added liquid viscosity does not affect the mixing time for the added liquid viscosities used in the experiments.

The adhesion property of the added liquid was found to have some influence. High viscosity additions containing PVP seem to be less likely to stick to the vessel wall or bottom than additions of sugar syrup are. This was not investigated further.
3.6 Practical Implications

The effect of density differences on mixing times is stronger than that of viscosity differences. For the geometry used here, mixing times for liquids of similar densities can be predicted with reasonable accuracy by \( N_{ct} \approx 30 \). This is valid for added liquid viscosities well into the region where in industry the addition would be premixed anyway. For liquids of similar viscosities, however, even small negative density differences can result in mixing in the gravity controlled regime. Depending on the liquids' properties and on the process conditions the mixing times can then be very long.

The chance of the added liquid surfacing or reaching the bottom also depends on the feed location. Addition near the stirrer shaft is preferable. If at all possible the liquid should be introduced near the stirrer. Adding the liquid in smaller portions or as an elongated stream is also advantageous.

For the stirrer controlled regime, scale-up is equal to that of the blending of liquids of equal physical properties. On the basis of the experiments no decision can be made about the position of the boundaries of the mixing regimes after scale-up. Furthermore, the gravity controlled mixing time has its own scaling rules that are, as yet, also unknown.

The added liquid volumes used in this study were small. In industrial situations this volume can be much larger so that gravity controlled mixing is more likely to occur. Therefore, in practice, the mixing problems found in this study can be larger. Additions with strong adhesive properties can also be expected to yield mixing problems.

As to the choice of the impeller, it is preferable to use a stirrer that produces flow rather than turbulence. This reduces the chance of the addition surfacing or clinging to the bottom. Increasing the stirrer rotational speed reduces not only the stirrer controlled mixing time, but also the chance of gravity controlled mixing.

3.7 Conclusions

The observations can be summarised as follows.

1. In the stirrer controlled regime—when liquid is added near the stirrer or when the bulk flow succeeds in transporting all of the added liquid to the stirrer—:
   a. the mixing time is practically independent of the viscosity ratio for \( 1 \text{ mPa\cdot s} \leq \mu_n \leq 5 \text{ Pa\cdot s} \);
   b. the mixing time does not depend on the location of injection;
   c. in the turbulent regime the mixing time is independent of probe position;
   d. for small \( V_a/V \), the mixing time is independent of the added volume;
   e. for very high added liquid viscosities, long mixing times can result because the added liquid is insufficiently deformed by the high shear in the stirrer region.
2. The probability for the added liquid to surface or to reach the bottom is affected by
   a. the position of addition;
   b. the density difference between the two liquids;
   c. the viscosity ratio;
   d. the stirrer speed.
   This probability is negligible in the *stirrer controlled regime*, and about 1 in the
   *gravity controlled regime*.

3. In the *gravity controlled regime*—when all or part of the added liquid surfaces or is
   added at the surface—:
   a. very long mixing times can result;
   b. the viscosities of both phases as well as the density difference determine the
      mixing time;
   c. the mixing time strongly depends on the amount of liquid that surfaces.

4. The situation of a high viscosity liquid that reaches the bottom is analogous to that of
   a buoyant liquid that surfaces. The time the addition remains on the bottom depends
   on its position on the bottom.

5. In the *intermediate regime*—when only part of the added liquid is transported to the
   stirrer—the mixing time is unpredictable and can be anywhere between the stirrer
   controlled mixing time and the gravity controlled mixing time.

6. Low viscosity additions deform into sheets, whereas high viscosity additions deform
   into threads. This complicates modelling, because a different model is needed in each
   case.

7. Mixing time measurements with an A310 stirrer show that $N \cdot t_m$ is about 1.8 times that
   of the PBT. The energy required for homogenisation for equal stirrer rotational speed,
   equal mixing time and equal power input is 0.36, 1.17 and 1.05 times that of the PBT,
   respectively. For a DT these energy ratios are 1.74, 0.56 and 0.82.

8. It is not possible to pronounce upon the position of the boundaries of the mixing
   regimes after scale-up on the basis of the available data. The scaling rules of the
   gravity controlled mixing time are, as yet, also unknown.

The absence of an influence of $\mu^*$ on the dimensionless mixing time in the stirrer
controlled regime implies that the deformation of the added liquid is not the limiting
factor in these blending processes. This is confirmed by the visualisation, which showed
that the deformation is very fast. This, combined with $N \cdot t_m$ being constant, shows that
the large-scale flow determines the mixing time, even for added liquid viscosities of up
to 5 Pa·s. It can be concluded that when all of the added liquid is transported to the
stirrer the homogenisation time depends on the rate of distribution of the added liquid
over the vessel.
Chapter 4—Blending Model

A model is described to simulate mixing operations in stirred vessels and predict mixing times. The simulation program MIXIM uses the flow field calculated by the Computational Fluid Dynamics program FLUENT to predict the chances of surfacing of buoyant additions, the circulation time and the mixing time. The model includes turbulence and buoyancy. An outline of the computer program MIXIM is given.

4.1 Introduction

The observations presented in the previous chapter show that when liquids of differing densities and viscosities are blended in stirred vessels, three mixing regimes can be distinguished.

1. In the stirrer controlled regime all of the added liquid is transported to the stirrer by the large-scale flow in the vessel. This includes those cases where liquid is deliberately added near the stirrer. In this regime the mixing time is equal to that of equi-viscous, neutrally buoyant additions for added liquid viscosities between 1 mPa-s and 5 Pa-s.

2. In the gravity controlled regime all of the added liquid either rises to the surface or reaches the bottom of the vessel and remains there until it is blended into the bulk by turbulent vortices. Depending on the properties of the liquids and on the stirring conditions this situation can yield very long mixing times.

3. In the intermediate regime only part of the liquid is transported to the stirrer, the amount depending on the bulk velocity at the moment of injection. Mixing times in this regime can be anywhere between those in the other two regimes.

These observations have implications for the modelling of the blending process. Clearly, the large-scale bulk flow at the position of injection determines which regime will occur. Furthermore, because no marked effect of viscosity ratio on mixing time is observed in the stirrer controlled regime, it can be concluded that the deformation and diffusion of the added liquid is fast compared with the rate of distribution over the vessel. This is confirmed by visualisation experiments, as will be made clear in this chapter. Therefore, it may be assumed that once a buoyant addition has been pulled down to the stirrer, the probability of surfacing owing to the density difference has become zero, because the dimensions of the addition are reduced to a scale where buoyancy effects are negligible\(^1\). This means that the modelling of the mixing process can

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\(^1\) For heavy high viscosity additions the chance of the liquid reaching the bottom may not become zero after one stirrer passage. However, this situation will not be examined here.
be divided into three parts:

- calculation of the probability of surfacing by calculating the trajectories of added fluid packages, taking into account buoyancy effects and deformation; this corresponds to determining the mixing regime: a small probability indicates the stirrer controlled regime, a high probability indicates the gravity controlled regime;

- given the situation of stirrer controlled mixing, calculation of the time needed for deformation and diffusion until the liquid is indistinguishable from its direct surroundings;

- calculation of the time needed for distribution of the partly blended solute over the vessel; for this step, buoyancy effects and deformation can be neglected, because after the previous step of deformation and diffusion the addition is sufficiently merged with its immediate surroundings.

A computer code, MIXIM (short for MIXing SIMulation), was written to simulate these steps. It calculates the trajectories of the added liquid, using the information about the three-dimensional flow field in the vessel that is supplied by the output files of the Computational Fluid Dynamics program FLUENT. For each point in time the next position of the added liquid package is predicted using a probabilistic Monte Carlo method based on the local turbulent velocity. With these trajectories the probabilities of surfacing and the time for distribution over the vessel can be calculated.

Essentially, this method can be applied for any vessel geometry or size and any combination of liquids. This would enable predictions about scale-up before the actual mixing equipment has been built.

The constituent subjects of the model will be discussed in the following order.

- Tracking of the Added Liquid
  - passive particles in turbulent flow
  - buoyant & settling particles in turbulent flow
- Deformation
  - deformation by the mean flow
  - deformation by the turbulent component of the flow
  - surface tension effects
  - viscosity effects
- Combined Effect of Deformation and Diffusion
- The Stirrer
- The Mixedness Criterion

Finally, the computer code based on this model, MIXIM, will be introduced.
4.2 Tracking the Added Liquid

The history of a drop\(^2\) of liquid added to the bulk of a stirred tank is determined by a combination of factors. Depending on the conditions in the vessel, the properties of the liquids and the position of the addition point, the drop may pass through several of four main zones: the stirrer region, the free surface, the bottom of the vessel, and the bulk. In each zone the drop can be deformed by or blended into the bulk fluid. In addition, from each zone the drop may be transported to another zone.

In the stirrer controlled regime, where all of the added liquid moves to the stirrer region, the blending process is reflected in the graphs of the measurements of conductivity against time, as shown in figure 4.1. The first peak marks the first passage of the added liquid along the probe. The second peak is much lower already, indicating that the added liquid has to some extent merged with the bulk liquid. In some cases a third peak is visible, but only vaguely, so within two or three circulations the added liquid, merged with its direct surroundings, can hardly be distinguished from the bulk liquid.

In the stirrer region the turbulence intensities as well as the shear forces are high, so that drops stand a good chance of being deformed. Drops may also be deformed by physical contact with the stirrer. Especially when the viscosity of the added liquid is very high compared with that of the bulk, the shear forces in this region are important for the mixing process, because in other parts of the vessel the shear forces may be too weak to cause large deformation.

In the bulk the shear stresses and the level of turbulence are lower, but deformed drops may be deformed further or be blended completely. For very high viscosity additions, however, the deformation rate will be too low, and longer mixing times will result.

The large-scale flow, combined with the net force resulting from density differences, determines whether or not a drop reaches the free surface or the bottom of the tank. If it does reach either place, the added liquid will generally remain there, provided the net

\[\text{conductivity}\]

\[0 \quad 50 \quad \text{N}t\]

**Figure 4.1. Typical conductivity response in the stirrer controlled regime.**

\(^2\)In the literature on miscible liquids the word *drop* is frequently used to indicate parts of the added liquid. In that case, as in this thesis, the word does imply neither immiscibility nor the presence of interfacial tension.
force is in the appropriate direction. The liquid can re-enter the bulk by turbulent eddies. This mechanism may yield mixing times that are long compared with those in the stirrer controlled regime, as was shown in figure 3.14.

The path a fluid particle will follow, and therefore the regions the particle will visit, can be predicted if the local turbulent velocities in the vessel are known. In the model described here the information about the flow in the vessel is provided by FLUENT. The output of this program is used to calculate the trajectories of the added liquid, taking into account the local values of the energy dissipation rate and the turbulent kinetic energy density. In all cases a one-way coupling is used: the added liquid is assumed not to affect the bulk velocities. This assumption is valid for small added liquid volumes.

The calculations have been done for passive and buoyant particles. More details about the FLUENT calculations can be found in chapter 2 and in Bakker (1992).

4.2.1 Passive Particles in Turbulent Flow

Total homogenisation of the vessel contents requires the distribution of the additive over the whole vessel. This large-scale mixing is mainly taken care of by the average flow field, but the turbulent component of the velocity field plays an important role as well. The contribution of the turbulence is the shifting of fluid elements from one streamline to another, which causes a stronger separation rate of initially neighbouring elements. If stagnant zones exist, turbulence is even essential for the exchange between these zones and the rest of the vessel.

The turbulence model used in the FLUENT calculations—the algebraic stress model—is three-dimensional and FLUENT enables the user to get information about the anisotropy of the turbulence. However, only the time-averaged values of the local turbulent kinetic energy $k$ and the local energy dissipation rate $\varepsilon$ are used, because MIXIM is based on an earlier version of FLUENT that does not supply this information. From the kinetic energy the standard deviation ('rms value') of the turbulent velocity fluctuations is therefore calculated by

\[ u_t = \sqrt{\frac{2k}{3}}. \]  

With this standard deviation the turbulent flow field in the vessel is modelled, assuming isotropic turbulence. A vector $r$ is created, composed of three normally distributed random numbers with an expectancy equal to zero and a standard deviation equal to unity. This vector is multiplied by the local value of $u_t$ to yield the three-dimensional instantaneous turbulent component of the velocity. This velocity, combined with the local mean velocity $\bar{u}(x)$, is then used to calculate the next position $x_{i+1}$ of an 'injected' drop by simple point slope integration:

\[ x_{i+1} = x_i + \Delta t (\bar{u}(x_i) + r u_t(x_i)) , \]  

where $\Delta t$ is the time step. Second-order Runge-Kutta integration was also applied, but
the differences in the results did not justify the extra calculation time needed for that method.

For each drop $r$ is kept constant during a time interval $\tau$, the maximum eddy lifetime, that is related to the local values of $k$ and $\varepsilon$ (see Creare x (1990)) by

$$
\tau = \frac{C^\mu}{\sqrt{\varepsilon}} \frac{k}{\varepsilon}.
$$

The constant $C^\mu$ is that used by FLUENT to calculate the effective turbulent viscosity (0.09). After this time a new $r$ is generated. If a drop migrates to another grid cell, $r$ remains the same until the eddy lifetime exceeds the new cell’s $\tau$.

The normally distributed random numbers are generated using the method described by Abramowitz & Stegun (1965). With a pair of uniform deviates $U_1$ and $U_2$, the normal random deviate

$$
x = \sqrt{-2 \ln U_1} \cos (2 \pi U_2)
$$

is formed. For the generation of the uniform deviates a method based on a generalised Fibonacci’s series is used:

$$
U_n = N_n/1000, \quad \text{with} \quad N_n = (N_{n-1} + N_{n-15}) \mod 1000.
$$

The method was tested for its long term behaviour and was found to be suitable for this application.

The time step for the calculation of the next position was different in each cell. Its value was proportional to the minimum value of $\tau$ and the cell dimensions divided by the three local mean velocities:

$$
\Delta t = \min(l_z/u_z, l_r/u_r, l_\phi/u_\phi) \tau/c,
$$

where $l$ is the cell length and $u$ the local mean velocity in the axial ($z$), radial ($r$) and angular/tangential ($\phi$) direction, and $c$ is a constant that was normally set to 2. The solutions proved to be sufficiently independent of $c$ for $c \geq 2$.

This way of modelling neglects the coherence that exists within turbulent flows. Firstly, neighbouring drops are assigned totally independent velocities, whereas in a real turbulent flow there is a correlation between the velocities of fluid elements that are close to each other: the smaller-scale eddies. Secondly, larger-scale velocity coherence is also absent from the model, because the calculated velocity field, even the turbulent part of it, is a time average. The absence of coherence on each of the two scales causes the drops to separate at a velocity that is too great. At this stage there is, however, no solution to this problem apart from keeping track of the distances between all the drops in order to correlate velocities of neighbouring drops. This would especially reduce the separation rate on the smaller scale. At the present level of computational power, however, this solution would render the simulation extremely slow. Future computer generations are expected to resolve this difficulty. The two problems should be kept in mind during the analysis of the rate of distribution over the vessel.

3Angular length, tangential velocity.
4.2.2 Buoyant and Settling Particles in Turbulent Flow

When a liquid has a lower density than the bulk to which it is added, it may rise to the surface of the vessel, where it may stay for some period of time. Liquids that are heavier than the bulk may settle and cling to the bottom of the vessel. Both situations can yield very long mixing times, as was shown in the previous chapter.

To take these effects into account, the Richardson number \( Ri \) could be used for the analysis of measurements (e.g. Rielly & Pandit (1988) and chapter 3). This number is a measure for the ratio of the potential energy density of the added phase and the kinetic energy density of the bulk phase. However, this approach only takes into account the overall effects of density differences. It disregards the effects of the feed position and the time-dependence of the flow.

A more fundamental approach to buoyancy effects is hampered by the fact that little is known about the rising or sinking velocity of deformed masses of liquid in another liquid. As the added drop is transformed into a very complex but still connected shape, buoyancy effects change.

However, for the more ideal situation of solid spheres and single-immiscible—drops various correlations for the steady state velocity relative to the surrounding fluid, \( u_{buoy} \), can be found in the literature. A survey of these is given by Wallis (1974). For a rigid sphere Wallis distinguishes four regions in the domain of a dimensionless radius

\[
r^* = r \left( \frac{\rho_0 \Delta \rho}{\mu_0^2} \right)^{1/3} \tag{4.7}
\]

and gives correlations for each region to calculate the dimensionless velocity for solid spheres:

\[
u^* = u_{buoy} \left( \frac{\rho_0^2}{\mu_0 \Delta \rho} \right)^{1/3} \tag{4.8}
\]

The coefficients for the correlation \( u^* = a r^{*b} \) are given in table 4.1. From this dimensionless velocity the actual value of \( u_{buoy} \) can be calculated. The rigid sphere approximation was used here because other methods require information about surface tension and the deformation caused by the drop’s relative velocity. The velocity calculated in this way deviates from that of a drop with a mobile interface by a factor of not more than four.

<table>
<thead>
<tr>
<th>( r^* )</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;1.5</td>
</tr>
<tr>
<td>1.5...10</td>
</tr>
<tr>
<td>10...36</td>
</tr>
<tr>
<td>&gt;36</td>
</tr>
<tr>
<td>----------</td>
</tr>
<tr>
<td>a</td>
</tr>
<tr>
<td>0.222</td>
</tr>
<tr>
<td>0.307</td>
</tr>
<tr>
<td>0.693</td>
</tr>
<tr>
<td>2.5</td>
</tr>
<tr>
<td>b</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>1.21</td>
</tr>
<tr>
<td>0.858</td>
</tr>
<tr>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 4.1. Coefficients for the correlation \( u^* = a r^{*b} \).
When a drop is released in a liquid, it will not immediately attain its terminal velocity relative to the surrounding liquid. To get an idea of the time scales involved, the time needed for a drop to reach 50% of its steady state velocity, \( t_{50\%} \), was calculated by a simple program. The drop was assumed to be a rigid sphere, with a diameter of \( d_d \) and a friction coefficient equal to

\[
C_f = \frac{24}{Re_d} + 0.43 ,
\]

with the drop's Reynolds number:

\[
Re_d \overset{\text{def}}{=} \frac{\rho_0 u d_d}{\mu_0} ,
\]

where \( u \) is the drop’s instantaneous relative velocity. For the calculation of the acceleration of the drop an added mass equal to \( \frac{1}{2} V_d \rho_0 \) was added to the drop’s own mass \( V_d \rho_d \):

\[
\frac{d u}{d t} = \frac{\left( \rho_0 - \rho_d \right) g V_d - \frac{1}{2} \rho_0 u^2 C_f \frac{\pi}{4} d_d^2}{\left( \rho_d + \frac{1}{2} \rho_0 \right) V_d} .
\]

As indicated above, the rigid sphere approximation is not correct, but the calculated times give a good impression of how quickly the terminal velocity is reached. Table 4.2 lists some examples. These times, together with the larger errors resulting from the lack of information about the form of the drop and interfacial effects, justify the approximation that a drop reaches its final velocity instantaneously. This results in an overestimation of the drop’s relative velocity. The assumption of a rigid interface, on the other hand, leads to an underestimation of this velocity.

<table>
<thead>
<tr>
<th>( \Delta \rho ) kg/m(^3)</th>
<th>( \mu_0 ) mPa·s</th>
<th>( d_d ) mm</th>
<th>( u_{\text{buoy}} ) mm/s</th>
<th>( t_{50%} ) ms</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1</td>
<td>1</td>
<td>6.1</td>
<td>54</td>
</tr>
<tr>
<td>10</td>
<td>1</td>
<td>10</td>
<td>52</td>
<td>434</td>
</tr>
<tr>
<td>100</td>
<td>1</td>
<td>1</td>
<td>34</td>
<td>32</td>
</tr>
<tr>
<td>100</td>
<td>1</td>
<td>10</td>
<td>172</td>
<td>144</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>10</td>
<td>34</td>
<td>311</td>
</tr>
<tr>
<td>100</td>
<td>10</td>
<td>1</td>
<td>5.5</td>
<td>5</td>
</tr>
</tbody>
</table>
The velocity calculated with Wallis' correlations, combined with the local mean and turbulent velocities, is used to calculate the next position of the drop (see figure 4.2):

\[ x_{t+1} = x_t + \Delta t \left( u(x_t) + r u_t(x_t) + u_{buoy} \right) . \]  

\[ (4.12) \]

\[ \text{Figure 4.2. Vectors used to calculate the next drop position.} \]

### 4.3 Deformation

Calculation of the deformation of drops would serve two purposes.

- In the first place the deformation, combined with diffusion, determines the small-scale mixing rate. As already mentioned in section 4.1, the measurements show that this deformation is rapid in the stirrer controlled regime. In that case it is not necessary to model the deformation.

- In the second place the deformation changes the effect of buoyancy: the rising or settling velocity of drops that are deformed by velocity gradients in the bulk flow will differ from that of the original drop. However, as mentioned in the previous section, the effect of the deformation on rising or settling velocities is not known.

Furthermore, visualisation shows that the mechanism of deformation depends on the viscosity of the added liquid (see section 3.3): low viscosity additions are deformed into sheets, whereas high viscosity additions are deformed into threads. It is as yet unknown which mechanism will prevail in a given situation. This seriously hampers the modelling of the deformation.

For these reasons the calculation of the deformation of the added drop was left out during the final calculations, which implies that in the simulation all drops retain their initial sizes. Nevertheless, since the program contains the algorithms needed for taking the deformation into account, the basics of the modelling of deformation are given here, first for the large scale, then for the small scale.
4.3.1 Deformation by the Mean Flow

Fluid packages larger than Kolmogorov’s length scale \( l_K \) are deformed by eddies of the scale of the packages. For relatively large packages or drops the deformation can be estimated using the gradients of the mean velocities. The deformation rate of a material line element (see figure 4.3) is given by:

\[
\frac{D}{Dt} \left( \frac{dx_k dx_k}{dx_m} \right) = \left[ \frac{\partial u_k}{\partial x_m} + \frac{\partial u_m}{\partial x_k} \right] dx_k dx_m. \tag{4.13}
\]

![Figure 4.3. Deformation of a line element.](image)

The deformation rate therefore depends on the orientation of the material line element. In general, the orientation of a deformed drop is not known, so the deformation rate cannot be calculated.

However, for simple cases of laminar elongational flows the rate of extension, defined by

\[
e = \frac{1}{s(t)} \frac{ds(t)}{dt}. \tag{4.14}
\]

(where \( s(t) \) is the distance between two points) is given by

\[
e = C_e \sqrt{\frac{\varepsilon}{V}} \tag{4.15}
\]

(Bolzern & Bourne (1983)). For axisymmetric elongation, \( C_e = 0.577 \); for planar extension (pure shear), \( C_e = 0.5 \); and for two-dimensional elongation, \( C_e = 0.289 \). The resulting deformations show an exponential growth:

\[
s = s(0) \exp \left[ C_e \sqrt{\frac{\varepsilon}{V}} t \right]. \tag{4.16}
\]

It is plausible to assume that for the mean flow in a mixing vessel \( C_e \) can be estimated by 0.5.

For laminar extensional flow in an incompressible fluid the local rate of energy dissipation in the mean flow per unit mass, \( \varepsilon \), is given generally by

\[
\varepsilon = 2\nu \sum_i \left| \frac{\partial u_i}{\partial x_i} \right|^2. \tag{4.17}
\]

This enables an estimation of the deformation caused by the mean flow by using the average velocities supplied by FLUENT for the calculation of \( \varepsilon \).
4.3.2 Deformation by the Turbulent Component of the Flow

When the mixing has been advanced to a scale of order $l_k$ the role of the deformation by the average flow is taken over by the deformation by the turbulent eddies. Fluid flow on the scale of those eddies does not 'know' its origin. The scales of length, time and velocity of those eddies—Kolmogorov's scales—depend only on the local energy dissipation rate and the kinematic viscosity.

Bolzern & Bourne (1983) show that an initially compact fluid element whose size is small compared with $l_k$ will be drawn out into a disc or lamina after a short time. Here, the thickness $d$ of the disc changes as

$$ d = d_0 \exp\left(-0.5\sqrt{\frac{\varepsilon}{\nu}} t\right) $$

(4.18)

(where $d_0$ is the initial thickness), but in this case the local eddy dissipation rate must be used for $\varepsilon$ rather than $\epsilon$ calculated from the mean flow. As shown in section 2.2.3, this local eddy dissipation rate varies as a function of place by several orders of magnitude.

Fluid packages with dimensions between the large scale and the smaller turbulent scales are deformed by both the mean flow and the turbulence. There is no model for this very complex three-dimensional deformation. The deformation rate might be estimated by taking the largest value of the local deformation rates on the large scale and on the small scale.

4.3.3 Surface Tension Effects

When miscible liquids are brought into contact, interfacial tension effects are almost absent. Smith & al. (1981) report measurements showing a comparatively low and declining interfacial tension between miscible oils. The measured tension was only about 1 mN/m when the liquids were first brought into contact and fell to less than one tenth of that value within about one minute. These findings are confirmed by experiments where drops are subjected to shear as in a Couette flow. The drops are deformed continuously until the filaments can no longer be distinguished by the naked eye. No break-up occurs, contrary to what is the case with immiscible liquids where interfacial tension prevents the addition from being deformed above a certain level.

These findings justify the assumption made in this thesis that there is no interfacial tension at all.
4.3.4 Viscosity Effects

The effect of differences in viscosity on the deformation of miscible liquids in flow fields in general is not fully understood. For Stokes flow and simple geometries the stretching can be calculated. Wilmot (1989) gives a method for the calculation of the stretching of thin inclusions in two-dimensional flows with pure shear and simple shear. The evolution of the inclusion can, in principle, be determined, but even in these cases further simplifications are necessary.

For immiscible liquids with interfacial tension $\sigma$, measurements show that for both low and high values of $\mu^* (\equiv \mu_d/\mu_0)$ the shear needed to cause break-up of drops, $\gamma$, is higher than for $0.1 < \mu^* < 1$, as described by Grace (1982) (see figure 4.4). This is expressed by the ratio of viscous to interfacial tension forces needed for break-up:

$$\frac{\gamma \mu_0 d}{\sigma} = \frac{19 \mu^* + 16}{16 \mu^* + 16}$$

(4.19)

The ratio rises sharply, especially if $\mu^*$ is larger than 1. As indicated above, for the miscible case the surface tension is much lower than in the immiscible case, which according to this theory would quickly result in break-up. In spite of this, the added phase is stretched without break-up, and blending is brought about by a continuous decrease of the added phase’s thickness and a consequently increasing diffusion.

De Bruijn (1989) confirms the findings of Grace and calculates the deformation of immiscible drops in time-dependent simple shear flows. For the miscible case, however, his numerical analysis cannot be used, because the interface becomes increasingly diffuse, especially during the later stages of the process.

The measurements presented in the previous chapter show that the deformation of the added liquids is fast, even for high viscosity ratios. In a 1 mPa-s bulk, liquids of up to 1 Pa-s are readily deformed, and in the stirrer region, liquids of 5 Pa-s are deformed fast enough so as not to cause longer mixing times. This means that Grace’s dependence for immiscible liquids is not applicable here. Moreover, it means that for the mixing time in the stirrer controlled region the deformation does not need to be modelled accurately. It suffices to show that the time needed for deformation and the subsequent diffusion is short.

![Figure 4.4. Drop breaking (after Grace(1982)).](image-url)
4.4 Deformation & Diffusion Combined

Homogenisation on the smallest scales can only be accomplished by diffusion. When the blending has reached scales smaller than \( l_K \), no further turbulent mixing occurs. From then on the only mechanisms at work are shear and diffusion. After a short time of shear the alternating layers of additive and bulk become thinner and diffusion gets faster because the same concentration difference acts over a shorter distance.

The effect of deformation on diffusion can be calculated analytically, but the analysis is complicated. As our purpose is to show that the time needed for deformation and diffusion is short compared with that needed to distribute the additive over the vessel, a simple model will be used here. It simulates the diffusion of a marker substance from a cylinder with decreasing diameter by means of penetration theory. The process is split up into two stages:

- In the first stage the cylinder—initial diameter \( d_0 \)—is deformed without diffusion during a time \( t_{\text{def}} \). The diameter of the cylinder after this time is given by
  \[
  d_1 = d_0 e^{-\alpha t_{\text{def}}} ,
  \]  
  (4.20)  
  where \( \alpha \) is the time constant determining the deformation rate.

- In the second stage, diffusion takes place without further deformation.

The diffusion in the second stage can be described using the Fourier number:

\[
Fo \equiv \frac{D t_{\text{dif}}}{d_1^2} ,
\]  
  (4.21)  

where \( D \) is the diffusion coefficient and \( t_{\text{dif}} \) the duration of the second stage. The average marker concentration, \( \langle C \rangle \), as a function of \( Fo \) can be calculated from a graph of the dimensionless average concentration \( C^* \) (\( \equiv \langle C \rangle / C_0 \)) versus the Fourier number as given by, for instance, Beek & Muttzall (1975). For times that are not too short (\( Fo > 0.01 \)) the relation between \( C^* \) and \( Fo \) is given by:

\[
\log C^* \approx -0.175 - 10 \cdot Fo
\]  
  (4.22)  

(the coefficients have been estimated from the Beek & Muttzall graph for cylinders). When \( Fo \) exceeds 0.2, \( C^* \) is lower than 0.01, i.e. less than 1% of the initial marker substance remains in the cylinder. This critical value of the Fourier number, \( Fo_{\text{cr}} \), will be used as a criterion for the mixedness in this calculation.

The more the cylinder is deformed during the first stage, the shorter \( t_{\text{dif}} \) will be. The total time needed for deformation and diffusion, equal to

\[
t_{\text{tot}} = t_{\text{def}} + t_{\text{dif}} ,
\]  
  (4.23)  

has a minimum as a function of \( t_{\text{def}} \). The minimum value \( t_{\text{cr}} \) is the time after which the critical Fourier number is reached.

The diffusion rate calculated in this way is overestimated because the penetration theory presupposes a constant concentration outside the cylinder, which implies greater concentration gradients than found in the real case. On the other hand, the calculation is
conservative for two reasons. Firstly, in the model there is no diffusion during the first stage, while during the second stage there is no deformation. Secondly, the deformation rate for fluid elements on scales smaller than \( l_c \) is much higher than the mean velocity deformation rate used here. This will further reduce the time needed for deformation and diffusion.

Moreover, in a real blending process, diffusion usually also affects the deformation, as the solute concentration may change the viscosity. The viscosity of water, for instance, rises almost exponentially with the concentration of PVP, a solute used in the mixing time experiments. It is very difficult to give a general rule for this behaviour, because each solute and solvent combination has a different viscosity versus concentration relation. It may be assumed, however, that this effect accelerates the blending process, at least when \( \mu^* > 1 \).

Figure 4.5 gives \( t_{cr} \) versus \( \alpha \) for several values of \( d_0; D = 1 \times 10^{-9} \text{ m}^2/\text{s} \). The values for \( \alpha = 1.4 \text{ s}^{-1} \) correspond to the reduction in diameter of the added liquid between figures 3.9 and 3.10, where \( \mu_0 = 1 \text{ mPa} \cdot \text{s}, \mu_a = 1.6 \text{ Pa} \cdot \text{s} \) and \( N = 2 \text{ s}^{-1} \). The figure shows that the time needed for the combined deformation and diffusion is short compared with the mixing time, even for lower values of \( \alpha \) (lower stirrer speeds or regions of low shear). Only for very low values of \( \alpha \) or large diameters of the added cylinder, \( t_{cr} \) is of the same order as \( t_m \).

![Graph showing deformation times](image)

**Figure 4.5. Total times for deformation followed by diffusion.**

### 4.5 The Stirrer

Because the stirrer is not explicitly modelled by FLUENT a separate treatment for stirrer passages is needed. The measurements show, however, that for viscosity ratios of up to 5000 the dimensionless mixing time in the stirrer controlled regime is independent of
\( \mu^* \). This means that the shear and the turbulence intensity in the stirrer region are so high that deformation combined with diffusion is short compared with the mixing time. For the modelling of blending this reduces the stirrer model to one simple statement: drops that pass the stirrer are immediately deformed to a scale that allows the leaving aside of viscosity effects in the modelling of the later stages of blending. For the calculation of trajectories, formula 4.2 is applied in the stirrer as well as in the bulk.

### 4.6 The Mixedness Criterion

After a stirrer passage, the only remaining time needed for homogenisation is that needed for the distribution of the additive over the vessel. In the mixing time measurements the vessel contents are considered mixed when the fluctuations in the conductivitiy response are smaller than a chosen value, for instance 10% of the total increase in conductivity. This can be simulated by tracking a large number \( n \) of fluid elements simultaneously and counting the number of elements that pass a chosen plane of the vessel (the 'probe'), for instance the area swept by the stirrer, during successive periods of time \( t_{\text{probe}} \). This modelling is only valid for the stirrer controlled regime, because in the other regimes part of the addition remains at the surface or on the bottom of the vessel for a period of time that is as yet unpredictable.

If the number of elements passing this 'probe' during \( t_{\text{probe}} \) is too small, however, the statistical fluctuations in the number of elements passing the probe during the final stage of mixing will be larger than the mixedness criterion. This means that homogeneity will never be achieved. This situation can be prevented by increasing either the area of the 'probe', or \( t_{\text{probe}} \), or \( n \). Increasing the area causes an averaging over a larger region, whereas the real probe is very small compared with the vessel size. Increasing \( t_{\text{probe}} \) causes time averaging of the probe signal that does not correspond to that in the actual mixing time measurements. Increasing \( n \) is the only remaining option, although this slows down the simulation considerably.

### 4.7 Simulation Code MIXIM

The mechanisms described in this chapter enable the prediction of important characteristics of the blending process such as the trajectories the added liquid will follow, the chances of surfacing of buoyant liquids, the circulation time and the mixing time. The simulation program MIXIM was written to include these mechanisms.

A simulation starts with the injection of a drop or a number of drops at a specific position in the vessel. The trajectories of the drops are calculated from a Lagrangian point of view, taking into account turbulence and buoyancy.
For the sake of concision the structure of MIXIM is given here in a highly simplified form in a pseudo-language.

READ calculated velocity field
FOR number of simulations DO
  initialise drop parameters
  {position, diameter}
  REPEAT
    FOR all drops DO
      IF new turbulent vector needed THEN generate \( r \)
      calculate new position
      {using 4.12}
      IF too close to surface THEN eliminate drop*      {drop has surfaced}
      IF passed stirrer THEN eliminate drop*         {drop has been mixed}
      IF passed stirrer THEN store circulation time**
      store number of drops that passed the stirrer**
      {probe simulation}
    DONE
  UNTIL no drops left OR time > time limit
  calculate probability of surfacing*
  END

The statements marked by * are only executed for buoyant additions. For that situation the probability of surfacing is calculated by dividing the number of drops that have surfaced by the total number of drops. With this probability the mixing regime can be predicted.

The statements marked by ** are only executed for neutrally buoyant additions, simulating the stirrer controlled regime.

The number of drops that pass the stirrer during each time interval, registered as a function of time, simulates a conductivity measurement. With this simulated response a prediction of the mixing time in the stirrer controlled regime can be made as described in the previous section. The stored circulation times are used for the prediction of the circulation time distribution.

4.8 Conclusions

The theories described in this chapter enable the calculation of some of the characteristics of blending in stirred vessels using the results of Computational Fluid Dynamics. Most of the theories were formulated for idealised systems, but they provide a good basis for predictions about practical apparatus.

The modelling of the mixing is done in a two-step process. Firstly, the mixing regime is determined by calculating the probability of surfacing of rigid added drops. Secondly,
if the mixing is stirrer controlled, the time needed for distribution of the addition over the vessel is calculated. The deformation of an added drop was shown to be fast enough to justify the omission of deformation and diffusion from the mixing model. For the calculation of the trajectories, buoyancy and turbulence are taken into account. It is assumed that the added liquid does not affect the flow field in the vessel. As this procedure can be used for any vessel size and geometry, scale-up predictions will be made possible.

The results of simulations using the computer program MIXIM will be presented and discussed in the next chapter. The results will also be compared with the measurements described in the previous chapter.
Chapter 5—Mixing Simulation Results

The results of simulations of the mixing in a stirred vessel are presented. Using the output of the Computational Fluid Dynamics program FLUENT, the trajectories of neutrally buoyant and buoyant additions are calculated by the simulation program MIXIM. In this way the probabilities of surfacing of buoyant additions can be estimated. The mixing time in those cases where all of the added liquid is transported to the stirrer is predicted correctly by simulating conductivity measurements. A hypothetical industrial size vessel is analysed using both FLUENT and MIXIM.

5.1 Introduction

This chapter presents sample results of a computer program that was specially written as part of this project to simulate the blending process of miscible liquids of different densities and viscosities in turbulently stirred vessels. The theories implemented in this program have been discussed in chapter 4. The program is based on the observations by means of visualisation and mixing time measurements that have been presented in chapter 3. They show that density differences in particular can give rise to longer mixing times. Viscosity differences play a minor role. In general, three regimes can be identified:

1. The stirrer controlled regime: all of the added liquid is transported to the stirrer and is deformed by the strong shear forces there. The resulting dimensionless mixing times \( Nt_m \) are about 30, as in the case of the blending of liquids of equal properties. For bulk viscosities of 1 mPa·s this holds for added liquid viscosities of up to 5 Pa·s.

2. The gravity controlled regime: for buoyant additions all of the added liquid rises to the surface and is mixed into the bulk by turbulent eddies close to the surface; settling additions sink to the bottom and are also mixed into the bulk by the eddies. In this regime the mixing times can be much longer than in the stirrer controlled regime, depending on the properties of the liquids and the process conditions.

3. The intermediate regime: only part of the added liquid is transported to the stirrer, the rest rises to the surface or reaches the bottom. Here the mixing times can be anywhere between those in the other two regimes.

Which regime will occur under given conditions depends on the flow field and on the properties of the liquids that are to be blended. Especially the mean, large-scale flow and the density difference between the liquids are of great importance, because they determine the chance that the addition reaches the surface. The mean flow causes each fluid element to pass through regions of high shear regularly. For this reason a strong mean flow is the most important factor in homogenisation. Only where fast chemical
reactions are concerned, a high level of turbulence in the bulk might be more important.

For mixing operations it is necessary to know when mixing times can occur that are longer than those in the stirrer controlled regime. In the gravity controlled regime this is likely to happen, especially for large added liquid volumes. The modelling described in the previous chapter aims at predicting the possible occurrence of gravity controlled mixing and other aspects of the mixing in stirred vessels. Models were presented for the simulation of the turbulent flow field, buoyancy effects, deformation and diffusion, and conductivity measurements. These models were used to write the simulation code MIXIM (short for MIXing SIMulation). MIXIM calculates the trajectories of drops\(^1\) injected in the vessel. The purpose is to estimate the chances of surfacing of buoyant additions and to predict the mixing time in the stirrer controlled regime. MIXIM uses the information about the flow field supplied by the output files of the Computational Fluid Dynamics (CFD) program FLUENT in the way described in the previous chapter. As it is also explained there, deformation was left out for the calculations presented here, so that the diameter of the added drops remains constant. Furthermore, it is assumed that the added liquid has no influence on the velocity field in the vessel.

For the stirrer controlled regime the mixing time can be predicted by determining the rate of distribution of the addition over the vessel. This is done on the basis of the calculated trajectories. For buoyant additions the trajectories can be used to predict the mixing regime that can be expected.

The calculation of drop trajectories can also be done using FLUENT's particle tracking facility, but a separate program has several advantages over this facility. These are listed in section 2.3. One important advantage is that short-cut methods can be used to calculate the flow for different scales and stirrer speeds. When FLUENT is used, the whole flow field must be recalculated for each scale and speed. This usually takes a long time: for the vessel under consideration here a single calculation took more than one week. Using a separate program an estimate of the flow field in geometrically identical vessels can very easily be made by keeping

\[
\frac{u}{ND} \quad \text{and} \quad \frac{\varepsilon}{N^3 D^2} \quad \text{constant} \tag{5.1}
\]

(\(u\): velocity; \(N\): stirrer speed; \(D\): stirrer diameter; \(\varepsilon\): local energy dissipation rate; the local kinetic energy density, \(k\), scales with \(u^2\)). These scaling rules are only valid under certain conditions (see chapter 2), but for conversion to cases that are not too dissimilar in scale and stirrer rotational speed the results are sufficiently reliable.

In this chapter, sample results of the MIXIM simulations are presented. The addition of neutrally buoyant particles will be discussed first, followed by an analysis of buoyant additions. Finally, an industrial set-up will be analysed.

\(^1\)In the literature on miscible liquids the word *drop* is frequently used to indicate parts of the added liquid. In that case, as in this thesis, the word implies neither immiscibility nor the presence of interfacial tension.

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In all cases, a pitched blade turbine (PBT) was used for the simulation. Except for the industrial size vessel, the simulated vessels are cylindrical vessels of 29 cm and 64 cm diameter, fitted with four baffles. The geometry of those vessels is given in figure 5.1. One three-dimensional case calculated by FLUENT was used for the cylindrical vessels: a 64 cm diameter vessel, filled with water and stirred at a rotational speed of 1 s$^{-1}$. For other situations the flow characteristics were calculated using the relations in formula 5.1.

For several reasons the conditions used for the simulations vary. In some cases the simulation was to be compared with actual mixing experiments, so the experimental conditions were reproduced as closely as possible. In other cases, the conditions were chosen because they produced clear illustrations. In still other cases there is no particular reason for the conditions used and other conditions could have been chosen just as well.

It is important to note that in this chapter two types of conclusions are drawn. In those cases where the simulation can be compared with actual data, as is the case with the probabilities of surfacing and the mixing time prediction, the conclusion applies to the predictive value of the simulation. Where verification of the calculations is not yet possible, however, as in the case of particle trajectories and Poincaré sections, the conclusions are about the mixing itself. These conclusions are only valid insofar as the simulation itself is reliable. From the fact that in the verifiable cases the simulation is correct, it can be concluded that it is very likely that in the other cases the simulation can also be trusted.

### 5.2 Neutrally Buoyant Additions

The history of drops of a neutrally buoyant liquid—flow followers—that are added to a stirred vessel is predicted by calculating the trajectories the drops will follow. Because the flow in the vessel is turbulent, all added drops will follow different paths. For each
feed position the probability that a drop is transported to the stirrer within a given period of time can be calculated by tracking a large number of drops that are injected at that position. Predictions of the circulation time can also be made on the basis of the trajectories.

5.2.1 Trajectories

The three-dimensional velocity field calculated by FLUENT was used to predict the particle paths by means of point slope integration:

\[ x_{i+1} = x_i + \Delta t (u(x_i) + r u_r(x_i)) , \]  

where \( x_i \) is the position of the particle at the \( i \)-th time step, \( \Delta t \) the time step, \( u \) the local mean velocity, \( u_r \) the local turbulent (root mean square) velocity, and \( r \) a vector constructed of three normally distributed random numbers (zero mean, unit standard deviation). A new vector \( r \) is generated after a time that is an estimate for the maximum eddy life time, based on the local energy dissipation and the local kinetic energy density. A more detailed description has been given in the previous chapter.

Figure 5.2 shows the paths of three arbitrarily chosen flow followers released halfway between the shaft and the vessel wall, 5 cm below the surface in a 64 cm diameter vessel; \( \mu_0 = 1 \) mPa·s. The simulation is continued until the flow follower has passed the stirrer or until the maximum simulated time (30 s) has expired. The injection position lies between two baffles. The simulation was done for \( N = 1 \) s\(^{-1}\), but these paths are also correct for other rotational speeds as long as the scaling rules in formula 5.1 can be assumed to be valid.

In the picture on the left the release is shown as seen by an observer watching a transparent vessel. In the middle picture, only the axial and the radial coordinates are

*Figure 5.2. Trajectories of flow followers released between two baffles; the circle indicates the injection position; left: as seen from outside the vessel; middle: axial & radial coordinates only.*
Mixing Simulation Results

**Figure 5.3. Trajectories of flow followers released between shaft and baffle;**
*the circle indicates the injection position; left: as seen from outside the vessel; middle: axial & radial coordinates only.*

shown. This figure shows that the random turbulent velocity component has a strong influence on the trajectories: one of the three simulated flow followers in this example is captured in a loop and does not pass the stirrer during the simulated time. In cases where the flow characteristics outside the stirrer region are insufficient to blend the additive with the bulk, this could cause mixing problems, as was shown in chapter 3. Addition of high viscosity liquids may then result in much longer mixing times because the added liquid remains in a zone with low shear for longer periods. But also in the case of low viscosity additions this randomness causes an unavoidable distribution of mixing times.

The same situation, but with the injection position between the shaft and a baffle, is shown in figure 5.3. The trajectories differ from those in figure 5.2, because the mean flow is directed towards the shaft rather than downwards. Here, again, the turbulent component causes the addition to follow different trajectories. The difference between the trajectories in figures 5.2 and 5.3 reflects the three-dimensionality of the mean flow in the vessel.

It should be noted that the number of trajectories shown here is too small to draw conclusions about the consequences for the blending process. However, the figures do make it clear that three-dimensional, not two-dimensional calculations are necessary in order to predict the blending in stirred vessels reliably. They also show that the feed position strongly influences the paths of the added liquid. This will be seen even more clearly in the case of buoyant liquids.

### 5.2.2 Poincaré Sections

Another impression of the three-dimensionality of the flow may be obtained by means of Poincaré sections: a fluid element is traced and each passage through a fixed surface,
for instance the stirrer plane, is marked. After a large number of passages the acquired pattern shows where liquid is exchanged frequently and where the liquid is more stagnant.

In figure 5.4, a Poincaré section of the stirrer plane in a 64 cm vessel is shown. The markers differentiate between fluid elements crossing the plane in the upflow and those going downwards. There is some three-dimensionality caused by the baffles. Between the region with upward crossings and that with downward crossings there is a distinct boundary. The fluid that moves downwards is confined within a radius of about 0.7 times the vessel radius. This radius agrees with that where the FLUENT output shows the division between upflow and downflow (see figures 2.5 and 2.6). It also corresponds to the radius for which the area enclosed by it equals the area outside it: this radius equals $2^{-1/2} \approx 0.707$ times the vessel radius. This means that the average upward velocity is about the same as that of the stirrer induced downflow.

In figure 5.5, the plane at 0.2·$T$ above the stirrer plane is given. Here, the three-dimensionality is much more pronounced than in the previous figure. The areas of upward and downward motion form a twisted cross, showing the effect of the angular dependence of the axial velocity. The plane at 0.2·$T$ below the stirrer plane is shown in figure 5.6. Near the centre of the vessel the liquid can be seen moving upwards as well as downwards, as can be seen in the separate figures of the centre part on the right. This is caused by the turbulence in the recirculation flow under the impeller.

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**Figure 5.4. Stirrer plane crossings.**
Figure 5.5. Crossings in the plane 0.2T above the stirrer.

Figure 5.6. Crossings in the plane 0.2T below the stirrer. The centre part is also shown on the right, where the downward and upward crossings are given separately.

5.2.3 Time before Stirrer Passage

The figures in section 5.2.1 show that the chance that the injected liquid misses the stirrer may depend on the feed position. The average time $\tau_{P1}$ between the injection and the first stirrer passage as a function of addition position is a good measure for this chance. That time, calculated from the tracking of 1000 drops for each position, is shown in figure 5.7. The drops are added at a depth of 7 cm in a 29 cm diameter vessel.
The shorter times are caused by flow followers going directly to the stirrer in most of the cases. Liquid added at positions with longer times has a larger chance of missing the stirrer. The figure shows that \( t_{P1} \) depends mainly on the radial position of the injection. Clearly the angular coordinate of the feed position is of minor importance for \( t_{P1} \), despite the effects of the three-dimensionality of the flow as shown in the figures 5.2 and 5.3.

Because the stirrer zone contains the highest shear rates and the highest levels of turbulence it would be profitable to find addition points where the added liquid has the shortest time \( t_{P2} \), the time between injection and the second stirrer passage. High viscosity additions that survived the first stirrer passage would then get a second chance to be deformed. The times \( t_{P2} \) were calculated for the same positions as in figure 5.7. The time between the first and the second stirrer passage \( (t_{P2} - t_{P1}) \) proved to be equal to \( 18 \pm 2 \) s, with no dependence on the radial and angular coordinates of the addition position. This means that the addition position only affects \( t_{P1} \). After one passage all information about the original position appears to be lost because of the shuffling of trajectories that takes place in the stirrer.

This is also reflected in figure 5.8, where the angular coordinate \( \varphi_2 \) of a downward stirrer plane crossing is plotted against this coordinate of the previous downward crossing \( \varphi_1 \), and in figure 5.9, where the same is done for the dimensionless radial coordinate.

There is some structure in the dot density in figure 5.8. However, this is caused only by the non-uniform distribution of the angular coordinates of stirrer plane crossings. The figure shows that for all \( \varphi_1 \) the density distribution of \( \varphi_2 \) is about the same, as indicated on the right, and vice versa, as indicated at the top. This means there is no correlation between one stirrer crossing position and the next. The dimensionless radial coordinate shows more correlation between successive crossings (figure 5.9). For instance, for \( r_1/R > 0.4 \) the next crossing has only a small chance of occurring at \( r/R < 0.2 \). However, the correlation is very low.

\[ \text{Figure 5.7. Times (in s) before first stirrer passage for injection in the plane at a depth of 7 cm; the stirrer turns clockwise, } N = 1 \text{ s}^{-1}, \mu_0 = 1 \text{ mPa} \cdot \text{s}. \]
Therefore, it is not possible to find an optimal feed position on the basis of the first two stirrer crossings. All this goes to show that the best way of preventing mixing problems resulting from high values of $\mu_3$ is to add liquid close enough to the stirrer to ensure rapid capture in the first place.

Figure 5.8. Angular coordinate of downward stirrer plane crossing versus same coordinate of previous crossing with rough indication of dot density.

Figure 5.9. Dimensionless radial coordinate of downward stirrer plane crossing versus same coordinate of previous crossing.
5.2.4 Circulation Time

Measurements of the time intervals between the crossings of the stirrer plane in a disc turbine stirred tank show these times to be log-normally distributed (Gavlak & Calabrese (1989)), which implies that the distribution is skew, with a very long tail on the right. This is an indication that the circulation time $t_c$ between two stirrer passages in a PBT stirred tank can also be expected to be skew.

Simulation of $t_c$ is done by recording the times between two passages through the impeller for a passive flow follower. In figure 5.10 the distribution of $Nt_c$ is shown for a 64 cm vessel, stirred at 1 s$^{-1}$ by a PBT. The horizontal resolution is 1 s; 75000 stirrer passages were recorded. As with the disc turbine, the distribution is skew, but in this case it is also bimodal. This bimodality exists because a fluid element does not necessarily move through the area swept by the stirrer blades every time it crosses the stirrer plane. The maximum on the left is caused by flow followers passing the stirrer on two consecutive circulations. In that case $Nt_c$ is about 7. The flow followers causing the second maximum pass the stirrer, miss the stirrer during the next circulation and return to the stirrer after the following circulation. In that case the dimensionless time between two stirrer passages is about 14. The figure shows that this happens in the majority of cases.

Although the modal value of $Nt_c$ is about 14, the broad distribution enables a mean value of about 20 (compare $t_{p2} - t_{p1} = 18$ s, previous section), while dimensionless circulation times longer than 20 have a probability of more than 30% to occur. As already mentioned, this may result in unexpectedly long mixing times when high viscosity additions are to be blended.

Again, mixing problems caused by high values of $\mu_a$ are most successfully avoided by adding the liquid at a position that ensures capture by the stirrer.

![Figure 5.10. Probability density function of dimensionless times between stirrer passages.](image)
5.2.5 Mixing Time Prediction

The measurements show that in the stirrer controlled regime the time needed for deformation and diffusion of the added liquid is short compared with the time needed for distribution of the partly blended addition over the vessel. Figure 5.11 illustrates this two-step process. The first step being fast, the prediction of the homogenisation time can be reduced to the simulation of the second step: distribution of liquid over the vessel. The physical properties of the tracer liquid can be assumed to equal those of the bulk liquid. It then suffices to determine the ‘self-distribution rate’ of the bulk using passive flow followers.

A number, \( n \), of infinitesimally small flow followers, simulating the partly blended addition after the first step in figure 5.11, were tracked simultaneously. The fraction passing the stirrer during 0.1 s intervals (\( t_{\text{probe}} \)) was registered as a function of time. This resulted in graphs of the form shown in figure 5.12, which was made using \( 10^4 \) particles injected at a depth of 6.4 cm in the 64 cm vessel at a radius of 16 cm, halfway between two baffles. The fraction \( P_{\text{probe}} \) (in %) of the particles passing the stirrer during each \( t_{\text{probe}} \) is plotted against the dimensionless time \( N \cdot t \). This graph resembles those of the conductivity measurements. However, there are two marked differences. Firstly, the circulations are more clearly visible, because the ‘probe’ is the total stirrer-swept area, not just a small probe. Secondly, the final statistical fluctuations are too large, so that small mixedness criteria cannot be used. The large fluctuations are caused by the relatively small number of flow followers. As mentioned in chapter 4, this can be prevented by increasing either the area of the ‘probe’, or \( t_{\text{probe}} \), or \( n \). Increasing the area or \( t_{\text{probe}} \) causes an averaging over a still larger region or a time averaging, respectively. Neither option resembles the real experimental conditions. The only possibility that was tried, therefore, is that of increasing \( n \).

Figure 5.13 shows the result of the same calculation with \( 10^5 \) particles. There the final fluctuations are much smaller. The dimensionless mixing time \( N \cdot t_m \) (mixedness criterion \( \Delta = 0.1 \)) in this case is about 27. To account for the difference in the value of \( \Delta \) between the experiments and the simulation, formula 3.1 can be applied, which overestimates the difference in \( N \cdot t_m \). This yields a dimensionless mixing time of 35.

Figure 5.11. Two steps in the mixing process.
Both 27 and 35 lie within one standard deviation of the measured value of $N \cdot t_m \approx 30$. Smaller values of $\Delta$ cannot be used in this simulation because of the fluctuations in the final signal. With $n=10^5$ the probability $p$ that a mixedness criterion of 0.1 is exceeded by these fluctuations within a 10 s interval is 0.92. Increasing $n$ reduces $p$. The simulation time, however, increases with $n$ and would have been about 40 hours for $n=10^6$.

The prediction of $N \cdot t_m \approx 30$ is more generally valid in the stirrer controlled regime, because the experiments show that density or viscosity differences have no effect in that regime. All PBT stirred vessels of the same geometry as that used here have about the same value for the dimensionless mixing time in the turbulent regime.

![Figure 5.12. Simulated conductivity response; $n = 10^4$.](image)

![Figure 5.13. Simulated conductivity response; $n = 10^5$.](image)
5.2.6 The Role of Turbulence

For the simulation of the conductivity measurements the turbulence was modelled as described in section 5.2.1. As noted in chapter 4, however, the dispersion rate is over-estimated in this model because all flow followers are assigned independent turbulent velocities, irrespective of the distances between them. In order to estimate the influence of turbulence on the mixing time the turbulent fluctuations were multiplied by a constant $C_t$:

$$x_{i+1} = x_i + \Delta t (u_i + C_t \cdot u_i(x_i)) ,$$

and the simulation of figure 5.13 was repeated. The dimensionless mixing times against $C_t$ are given in figure 5.14, which shows that above a certain level of turbulence an increase of turbulence intensity will not necessarily lead to faster blending. This can be explained by the chaotic nature of the mean flow in the vessel. Small differences in starting positions produce completely different particle tracks. This is true even if only the mean flow is considered: very simple laminar flows may result in chaotic mixing if the streamlines of the flow diverge (Ottino (1989)). The role of turbulence is mainly to distribute the added liquid over different streamlines of the mean flow, after which the diverging mean flow will take care of the further separation of the fluid elements. Above a certain level, an increase in the turbulence intensity will not result in a further improvement of the distribution rate.

![Graph](image)

*Figure 5.14. Predicted mixing time versus $C_t$. The value of $N \cdot t_m$ for $C_t = 0.2$ was too high to be simulated.*
5.3 Buoyant Additions

The simulation of the blending of buoyant additions was divided into two steps:
1. determination of the mixing regime by calculating the probability of surfacing for added drops: a low probability of surfacing corresponds to stirrer controlled mixing;
2. for those cases that show stirrer controlled mixing: calculation of the mixing time (the gravity controlled regime and the intermediate regime have not been modelled).

It is assumed that the addition, after having been drawn into the impeller region, has the same physical properties as the surrounding liquid (see also section 4.1). Therefore, the calculation of the second step is identical to that in the neutrally buoyant case, as in section 5.2.5, and will not be repeated.

5.3.1 Trajectories

Buoyancy was modelled by adding the steady-state rise velocity of the drop, $u_{buoy}$, as given by Wallis (1974) for solid spheres (see section 4.2.3), to the local instantaneous bulk velocity:

$$ x_{i+1} = x_i + \Delta t (u(x_i) + r u_i(x_i) + u_{buoy}) $$

(5.4 = 4.13)

This is only valid if the velocity of the drop relative to the bulk liquid is always equal to $u_{buoy}$. Because of inertia effects this is not the case. However, calculations showed that the times needed for the drop to reach 50% of $u_{buoy}$ are small (see the previous chapter).

Sample trajectories of buoyant drops of 6 mm diameter in the 64 cm diameter vessel are given in figure 5.15. The density difference ($\Delta \rho \equiv \rho - \rho_0$) is $-70 \text{ kg/m}^3$; $\mu_0 = 10 \text{ mPa s}$; $N = 3 \text{ s}^{-1}$. These values correspond to those in the measurements presented in

![Figure 5.15. Trajectories of buoyant drops released between shaft and baffle; the circles indicate the injection positions: $\Delta \rho = -70 \text{ kg/m}^3$; $\mu_0 = 10 \text{ mPa s}$; $N = 3 \text{ s}^{-1}$.](image)
figure 3.22. The injection distances from the axis are 0.2, 0.4 and 0.6 times the vessel radius $R$, respectively. Injection at the position closest to the axis results in all drops being pulled down into the stirrer. Addition near the baffle leads to the gravity controlled regime. From the middle position drops go either to the stirrer or to the surface. This difference between the three injection positions is found in the measurements as well as in the simulations.

The figure suggests that the position of injection determines the probability of surfacing of the added liquid. This will be analysed further in the next section.

5.3.2 Probability of Surfacing

The added drop’s probability of surfacing was simulated using MIXIM and compared with the results of FLUENT’s particle tracking facility and with some of the observations presented in chapter 3.

FLUENT’s particle tracking routine enables the user to calculate the paths followed by particles in the vessel. There is one fundamental difference between the algorithm used by FLUENT and that used by MIXIM. FLUENT uses the equations of motion for particles including drag, and calculates the resulting velocity. MIXIM, on the other hand, assumes that particles always move with their steady-state velocity relative to the surrounding liquid, thereby neglecting acceleration caused by the inertia of the drop. In chapter 4 it was shown that the time before a drop achieves 50% of its steady-state velocity is of the order of 5 to 500 ms. This implies that the error caused by neglecting the acceleration may be small. The two ways of calculating the trajectories will now be compared by examining the resulting probabilities of surfacing.

The comparison between FLUENT’s particle tracking on the one hand and MIXIM’s results on the other was made for three drop diameters. In this example the addition positions were between the shaft and a baffle in the 64 cm vessel, at radial distances of 0.2, 0.4 and 0.6 times the vessel radius. The density difference was $-100$ kg/m$^3$, the stirrer rotational speed was 1 s$^{-1}$. For each addition position 1000 drops were added. Each drop was tracked until it either reached the surface or passed the stirrer. The number reaching the surface was registered. Figure 5.16 shows the 90% confidence intervals of the probabilities of surfacing. The values predicted by both programs are almost equal. Those predicted by MIXIM are a little higher, owing to the steady-state velocity assumption. The difference is small, however, indicating that the steady-state velocity assumption yields satisfactory results.

The probability of surfacing increases with increasing drop diameter. This is caused by the stronger buoyancy forces for larger drops. The figure also shows that the probabilities of surfacing increase near the vessel wall. There, the mean flow is directed upwards, whereas closer to the shaft it is directed downwards.
Figure 5.16. Comparison between the probabilities of surfacing calculated by MIXIM and FLUENT. Injection 5 cm below the surface in a 64 cm vessel; \( \mu_0 = 1 \text{ mPa}\cdot\text{s}, \Delta \rho = -100 \text{ kg/m}^3; N = 1 \text{ s}^{-1} \).

Figure 5.17 shows the predicted probabilities of surfacing \( p_s \) as a function of stirrer rotational speed for 3 cm\(^3\) drops injected in the 29 cm vessel. Drops were added 10 cm below the surface at a radius of 10 cm, 5° behind a baffle. The probabilities are given for density differences of -5, -10 and -15 kg/m\(^3\). Below the graph the approximate positions of the boundary between the stirrer controlled regime and the intermediate regime are indicated for experiments with drops of high viscosity—which means small deformation of the added liquid—that are added at the same location in the vessel (see figure 3.20). These boundary positions correspond with the stirrer speeds that have a predicted probability of surfacing of about 40 to 50%. This suggests that for high viscosity additions the transition from the stirrer controlled regime to the intermediate regime may be predicted by calculating the stirrer speed that produces a 50% probability of surfacing.

Figure 5.17. Predicted probabilities of surfacing versus stirrer rotational speed. The arrows below the graph indicate the approximate positions of the transition between the stirrer controlled regime and the intermediate regime in the measurements for the three density differences; drop volume: 3 cm\(^3\); \( \mu_0 = 10 \text{ mPa}\cdot\text{s} \).
Figure 5.18 gives the probabilities of surfacing as a function of injection position in a plane at a depth of 7 cm in the 29 cm vessel. At each position 1000 drops were injected with a volume of 3 cm³ and a density difference of -15 kg/m³. Inside the plane, the probabilities mainly depend on the radial coordinate r (compare figure 5.15). In the angular direction the probabilities do not differ by more than a factor 2, in spite of the differences in the flow pattern with respect to that direction.

The probabilities of surfacing in the plane midway between two baffles are shown in figure 5.19. The probability of surfacing increases as the feed position is closer to the surface or the vessel wall. In those areas the mean flow is not directed downwards, giving the added liquid a better chance of escape. Addition of buoyant liquids in these areas is inadvisable.

Figure 5.18. Probabilities of surfacing for 3 cm³ drops in the plane at a depth of 7 cm; the stirrer rotates clockwise, $\mu_0 = 10$ mPa·s, $\Delta \rho = -15$ kg/m³, $N = 3$ s⁻¹.

Figure 5.19. Probabilities of surfacing for 3 cm³ drops in the top part of the plane midway between two baffles; $\mu_0 = 10$ mPa·s, $\Delta \rho = -15$ kg/m³, $N = 3$ s⁻¹.
Figure 5.20. Dimensionless times $(N \cdot t_{P1})$ before the first stirrer passage for injection of 3 cm$^3$ drops in the plane at a depth of 7 cm; the stirrer turns clockwise;

$\mu_0 = 10$ mPa·s, $\Delta \rho = -15$ kg/m$^3$, $N = 3$ s$^{-1}$.

In the region labelled 'undefined' no drops reach the stirrer.

As was the case with the flow followers, the feed position determines the path of the added liquid. In the buoyant situation, however, added liquid surfacing is undesirable because it may result in much longer mixing times.

5.3.3 Time before Stirrer Passage

As in the case of flow followers (figure 5.7) the time between injection and the first stirrer passage, $t_{P1}$, was calculated as a function of $r$ and $\varphi$ by tracking 1000 drops for each position. Figure 5.20 shows these times, made dimensionless, for $N = 3$ s$^{-1}$ and $\Delta \rho = -15$ kg/m$^3$. For almost all positions $N \cdot t_{P1}$ is somewhat longer than in the neutrally buoyant case, because the drops rise against the downward flow. The average difference is 2.5, which is lower than the standard deviation in the measured dimensionless mixing times. Here, as in the neutrally buoyant case, the dependence on $r$ is much stronger than that on $\varphi$. From some of the positions near the wall all the added drops rise to the surface, so no $t_{P1}$ could be calculated there. In the figure this is indicated by the area labelled 'undefined'. Because the probability of surfacing is higher near the wall, adding liquid there is inadvisable, especially as buoyant additions can give rise to longer mixing times when they reach the surface.

5.4 An Industrial Case

The procedure to be used in designing new vessels can be illustrated from the calculations done for an industrial size vessel. The case was set up to get some idea about the flow conditions in a larger vessel and the mixing problems that can be expected there. First, the equipment is chosen. Then the flow field is calculated using FLUENT. This information is used by MIXIM to make predictions about the probabilities of surfacing.
5.4.1 The Equipment

The vessel geometry, shown in figure 5.21, was synthesised from examples of industrial mixing equipment. The vessel measured 4.8 m by 2.0 m with a height of 2.0 m and was fitted with three 40 cm diameter PBT's on different shafts, dividing it into three identical imaginary compartments each with $H/T = 1.2$. The viscosity of the bulk liquid was 400 mPa·s and the bulk density 1500 kg/m$^3$. The stirrer rotational speed was 16 s$^{-1}$ ($Re = 9600$), so the total power input would be about 20 kW, corresponding to 0.7 W/kg.

5.4.2 FLUENT Calculations

The flow in the vessel was calculated using FLUENT. As with the laboratory vessels, these calculations were done by Bakker. A uniform grid of 24200 (22×22×50) cells was used and again the turbulent stresses were modelled using ASM. The impellers were modelled less precisely than those of the laboratory scale vessels in that, below the impeller, a uniform axial velocity profile was imposed as boundary condition and the tangential components were a linear function of the radial distance. The stirrer shafts were not modelled.

A first attempt, with all three stirrers rotating clockwise as seen from top, failed because the mean flow appeared to be unstable. During the FLUENT iteration process a large-scale oscillation occurred, which would have required a time-dependent simulation. This was not attempted, because the simulation code MIXIM was not designed for calculations with time-dependent flow fields. Moreover, the computational time needed for both the time-dependent FLUENT calculations and an adapted version of MIXIM would have been far too long for practical use.

![Figure 5.21. The industrial size vessel geometry.](image)
A solution was found in letting the middle stirrer revolve anticlockwise, still with downflow. In the real situation this would have implied replacing the stirrer by its mirror image. The calculation of the mean flow in the new situation converged on a steady solution.

Figure 5.22 shows the horizontal velocities in a plane just below the surface. Contrary to expectations, the flow pattern is not symmetrical. The vortices generated by the stirrers do not coincide with the positions of the shafts. The vortex on the left would appear to be stronger than the other two. The figure shows that, as far as the flow is concerned, the three 'compartments' cannot be treated as independent vessels with identical flow patterns.

The velocities in the plane through the stirrers are given in figure 5.23. As in the case of a single vessel, the flow in the vicinity of the stirrers is strong. However, the flow between the stirrer shafts is upwards, so liquid added there is not immediately transported to the stirrer plane. This can give rise to mixing problems in the case of buoyant

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**Figure 5.22.** Flow in a large vessel, calculated by FLUENT; top view; the centre stirrer rotates anticlockwise.

**Figure 5.23.** Flow in a large vessel, calculated by FLUENT; side view.
additions, as we will see in the next paragraph.

The velocity field calculated in this example can be expected to be generally reliable. Because of the crude modelling of the stirrers, however, smaller-scale phenomena may be absent in the calculated field. For instance, there are no recirculation loops beneath the impellers, although they can be expected in the real situation. Therefore, caution should be exercised in the interpretation of the details of the flow field.

5.4.3 Implications for Mixing

In figure 5.24 the probabilities of surfacing, \( p_s \), are given for 3 cm diameter drops of very high viscosity—which means there is no deformation—and a density of 1000 kg/m\(^3\) (so that \( \Delta \rho = -500 \text{ kg/m}^3 \)), added 20 cm below the surface. For each feed position 1000 drops were added. The value of \( p_s \) for the feed position above the middle stirrer could be calculated because the shafts were not modelled.

For this vessel, as in the case of the laboratory vessel, the probability of surfacing is highest near the wall. Because of the upward flow between the stirrer shafts, the probability of surfacing is also high there. The distributions of probabilities around the stirrer shafts are not identical for the three stirrers, because of the asymmetry of the flow. The best feed positions lie close to the shafts of the outer stirrers. The left stirrer has the best chance of capturing additions: the values of \( p_s \) are lowest there and the area where the chances are low is larger. In practice, however, it is impossible to foresee which stirrer will behave like the 'left stirrer'. The asymmetry in the flow will be established during the random start-up of the mixing by the stirrers.

When liquid is added at the surface, as is customary in many branches of industry, the chances of longer mixing times are, of course, much higher. As was shown in

\[<20\% \quad 20\ldots50\% \quad >50\%\]

**Figure 5.24. Probabilities of surfacing in the production size vessel (top view).**

*Injection of 3 cm diameter drops, 20 cm below the surface; \( \Delta \rho = -500 \text{ kg/m}^3 \).*

*The circles indicate the stirrer positions.*
chapter 3, even small density differences can then give rise to unexpectedly long mixing times. Injection in the bulk, preferably close to the stirrer, is therefore always advisable with buoyant additions.

The oscillations that appear to occur when the stirrers rotate in the same direction may have two effects. The instability is an effective way of preventing dead zones. This can reduce the mixing time. On the other hand, if there are large density differences the mixing time may become unpredictable because the chance that the additive remains on or reaches the surface is dependent on the velocity at the time and place of addition. This would be undesirable from the process operators’ point of view.

5.5 Discussion

The results presented in this chapter show that some of the mixing characteristics of a stirred vessel can be successfully analysed by means of the CFD program FLUENT complemented by MIXIM. This offers new possibilities for the design and scale-up of mixing apparatus, because predictions can be made before test equipment is built.

It is, for instance, possible to predict where zones with upward velocity will occur, so that these regions can be avoided when buoyant liquids are added. Further research will make clear how the chances of surfacing could be translated directly into a prediction of the mixing regime. Comparison between actual and simulated mixing processes will show what minimum level of shear stress and turbulence is allowable in the more stagnant zones for very high viscosity additions.

The model as a whole opens up new perspectives for simulation and an extended version of the simulation program will prove very useful. The development of such a comprehensive model would have to take into account the following aspects.

• The deformation of the added liquid by the bulk requires further theoretical and experimental study, because this deformation has implications for the estimation of the mixing time as well as for the velocity of the added liquid relative to the bulk flow.

• The relative velocity cannot be predicted satisfactorily in the case of a deformed drop.

• The modelling of the turbulence neglects the coherent structures of turbulence. This falsely enhances the distribution rate of the addition.

• Because the stirrer is not modelled explicitly, there is no way of predicting the deformation within the stirrer.

• The present simulations only include a PBT. Other stirrers should be examined as well.

• For larger added liquid volumes the assumption that the bulk flow is not affected by the addition does not hold. A much more complex, perhaps iterative, procedure should
be used in that case.

New generations of CFD programs can be expected to solve some of the problems existing at this moment. It will be possible to simulate the stirrer explicitly. This will enable the user to try out new stirrer designs and to predict the deformation of the added liquid within the stirrer. Moreover, time-dependent calculations will simulate turbulence more accurately than is possible at present. Full two-phase flow modelling will eventually provide better predictions of the combined deformation and buoyancy.

5.6 Conclusions

Mixing in stirred vessels was simulated using a combination of CFD and the program MIXIM.

- Neutrally buoyant additions
  - Particle trajectories and Poincaré plots show that it is essential to use three-dimensional flow fields for the analysis of mixing in stirred vessels.
  - The effect of the angular coordinate of the feed position on mixing characteristics is smaller than that of the radial coordinate.
  - Mixing times for neutrally buoyant additions—stirrer controlled mixing—can be predicted by simulating conductivity measurements. The calculated value \( N \tau_m \approx 30 \) is equal to that measured for a wide range of liquid properties, vessel sizes and stirrer speeds.
  - The circulation time distributions are bimodal and skew. The bimodality is caused by fluid elements passing through the stirrer plane but missing the stirrer. The skewness enables long circulation times that can give rise to mixing problems in the case of high viscosity additions.
  - There is no correlation between the angular coordinate of a downward stirrer crossing and the angular coordinate of the next crossing; for the radial coordinate the correlation is very small.
  - Turbulence is essential for the mixing time, but only up to a certain level. Above that level, increasing the turbulence intensity does not contribute substantially to shortening the mixing time.

- Buoyant additions
  - The mixing regime can be predicted by calculating the probabilities of surfacing for non-deforming drops. High probabilities correspond to gravity controlled mixing in the experiments, whereas low probabilities correspond to stirrer controlled mixing. The probabilities depend on the feed position: the closer this is to the vessel wall or to the surface, the higher the probabilities.
  - In the stirrer controlled regime, large-scale distribution of the partially blended
addition determines the mixing time. This implies that these mixing times can be predicted without taking into account buoyancy and viscosity effects. The prediction of the mixing times in this regime is therefore equal to that for neutrally buoyant additions.

◊ The mean flow in an industrial size vessel mounted with three impellers appears to be asymmetric, and is likely to be strongly time-dependent. This means that mixing times can be unpredictable in the case of buoyant or settling additions.
Chapter 6—Concluding Remarks

This chapter presents the general conclusions and lists the practical implications of this study. Additional measurements and model extensions are proposed.

6.1 General Conclusions

Three mixing regimes can be distinguished in the turbulent blending of liquids of differing densities and viscosities in stirred vessels.

- The stirrer controlled regime: all of the added liquid is added near or transported to the stirrer, where it is deformed rapidly. The time needed for the combined deformation and diffusion of the added liquid is short compared with the time needed for the distribution of the addition over the vessel. The effects of viscosity and density differences are negligible, and the well-known correlation for equiviscous, neutrally buoyant additions—\( N \cdot t_m \approx 30 \)—can be used for added liquid viscosities up to 5 Pa·s (bulk viscosity 1 mPa·s). Higher added liquid viscosities may result in very long mixing times because the shear rates in the stirrer region are incapable of deforming the added liquid. Higher bulk viscosities do not affect the mixing time, as long as the flow in the vessel remains turbulent. In the turbulent regime the mixing time is independent of feed position and probe position.

- The gravity controlled regime: all of the added liquid either rises to the surface or reaches the bottom of the vessel and remains there, under the influence of the density difference, until it is blended into the bulk by turbulent eddies. Depending on the stirring conditions in the vessel and on the properties of the liquids, this process may yield mixing times that are very long compared with those in the stirrer controlled regime. A small density difference by itself may cause gravity controlled mixing, whereas small viscosity differences unaccompanied by density differences do not.

- The intermediate regime, between the other two regimes: only part of the liquid is transported to the stirrer. The turbulent bulk velocity at the moment and the position of injection determines the amount of liquid that reaches the stirrer. This amount, in turn, determines the mixing time, which can take any value between the mixing times in the other two regimes. The relative standard deviation in the measured mixing times is largest in this regime.
Chapter Six

Which mixing regime occurs in a given situation depends on the probability of the added liquid surfacing or reaching the bottom of the vessel. This probability depends on the feed position, the density difference between the two liquids, the viscosity ratio and the stirrer speed. In the stirrer controlled regime the probability is negligible, whereas in the gravity controlled regime it is about 1. Scaling rules for the position of the boundaries of the mixing regimes are as yet unknown. However, the probabilities of surfacing can be calculated on the basis of the three-dimensional flow field as calculated by Computational Fluid Dynamics programs. This offers the possibility of predicting the mixing regime for mixing equipment in advance.

In the stirrer controlled regime the deformation in the stirrer region is very fast, so that the addition quickly merges with its direct surroundings. The resulting mixing is independent of viscosity or density differences, and can be modelled by simulating the distribution over the vessel of fluid elements that have the same properties as the bulk liquid.

A Lightnin A310 stirrer was compared with a pitched blade turbine (PBT). The dimensionless mixing times are about 1.8 times those of the PBT, but the energy required for homogenisation at the same stirrer rotational speed is about one-third of that of the PBT. In order to achieve the same mixing time as with the PBT, however, the A310 would require 1.17 times the energy needed with the PBT. Therefore, if a short mixing time is not the first requirement the A310 is more efficient, but when the mixing time is fixed the PBT is preferred. The energy required for homogenisation at equal power input is the same as that of the PBT.

For a disc turbine in the turbulent regime the energies needed for homogenisation at equal stirrer rotational speed, equal mixing time and equal power input are 1.74, 0.56 and 0.82 times those of the PBT, respectively.

A combination of CFD calculations and a purpose-written program, MIXIM, was used to simulate some important elements of the mixing process. The following conclusions can be drawn from the simulations.

- Particle trajectories and Poincaré sections show that a reliable analysis of the mixing process in stirred vessels calls for three-dimensional flow calculations.

- The probabilities of surfacing for non-deforming buoyant drops depend on the feed position. Small probabilities predicted by the simulation (<50%) correspond to stirrer controlled mixing in the measurements; larger probabilities correspond to the intermediate or gravity controlled regime.

- Although the flow in the vessel is three-dimensional, the probabilities of surfacing
mainly depend on the vertical and radial coordinates of the feed position. The probabilities increase near the vessel wall and near the surface, because the mean bulk flow is not directed downwards there.

- The effect of the angular coordinate of the feed position on the time between addition and the first stirrer passage is smaller than that of the radial coordinate. Near the vessel wall the times are longer than near the shaft.

- The circulation time distributions are bimodal and skew with a long tail on the right. Fluid elements that pass through the stirrer plane but miss the stirrer cause this bimodality. Although the modal value of the dimensionless circulation time \( N\tau_c \) is about 14, its mean value is about 20. In the case of additions of high viscosity—where the deformation of the added liquid in the stirrer region is essential for the blending process—the long circulation times can cause mixing problems.

- In the stirrer controlled regime, mixing times can be predicted by simulating conductivity measurements. This is done by tracking a large number of fluid elements starting from the feed position and counting the number of them that pass a chosen area (the 'probe') during each time step. The predicted value of the dimensionless mixing time \( N\tau_m \approx 30 \) equals that of the usual empirical correlation.

- Above a certain level of turbulence, the mixing time is not substantially shortened by a further increase of the turbulence intensity.

- The analysis of a rectangular industrial size vessel mounted with three stirrers shows that the mean flow in the vessel is not symmetrical and is probably time-dependent. In the case of buoyant or settling additions this may lead to unpredictable mixing times.

- Most of the theories that were used in the simulations were formulated for idealised systems, but they provide a good basis for predictions about real and therefore more complex apparatus.

### 6.2 Practical Implications

The blending of liquids of differing viscosities and densities should present no problems if the bulk flow transports the addition to the stirrer. This holds even for very high values of the viscosity ratio. The mixing times in that case are determined by the rate of distribution of the added liquid over the vessel: the usual correlations of the dimensionless mixing time versus the Reynolds number for the blending of liquids of about equal properties can be used.

When all or part of the added liquid surfaces or clings to the vessel bottom or wall, however, much longer mixing times can result, depending on the properties of the
liquids and the flow conditions in the vessel. This situation is undesirable in practical blending operations. Some measures that can be taken to prevent gravity controlled mixing are presented here.

• Small density differences can have a strong effect on the mixing time, whereas small viscosity differences cannot. This implies that, especially when liquids of differing densities are to be blended, the stirrer should be designed for strong flow rather than for turbulence, so that the bulk flow will transport all of the addition to the stirrer. Another possibility is pre-mixing of the addition, a procedure that is generally used only in cases with viscosity differences.

• The viscosity ratio has a smaller influence on the mixing time than the density difference. High viscosity additions can yield long mixing times when they surface or reach the bottom or the walls because of a density difference. Additions of very high viscosities can yield long mixing times regardless of the trajectory of the addition. In practical situations, however, these additions would be premixed anyway.

• The position of the feed point has a strong influence on the mixing regime (stirrer controlled, intermediate or gravity controlled). Close to the shaft the chance of gravity controlled mixing is smaller than close to the vessel walls, due to the strong downward flow of the bulk liquid. Addition in smaller portions can be advantageous: buoyancy effects are reduced, so that the liquid is more likely to be transported to the stirrer.

There are no simple scale-up rules for the mixing of liquids of differing densities and viscosities. For the stirrer controlled regime the mixing times can be expected to obey the rule of a constant dimensionless mixing time. Flow simulation and analysis can be expected to be able to predict whether stirrer controlled mixing occurs or not.

6.3 Further Investigations

The experiments presented here could be extended and the proposed model can be improved. The most important points are listed here.

• Mixing time measurements and visualisation experiments in vessels on a larger scale and with other stirrer types would provide information about the boundaries of the mixing regimes and their scale-up rules.

• Measurements in the gravity controlled regime will provide information about the mixing rate in that regime and a separate model should be developed for the prediction of mixing times. In combination with the predicted probabilities of surfacing this would yield mixing time predictions for a wide range of process conditions.

• The turbulent part of the velocity field is at present modelled very crudely. Coherence in the velocity field—correlation between fluid elements that are close to each
other—and anisotropy should be incorporated in the model.

- Buoyancy effects and deformation rates for deformed drops and larger masses of added liquid are as yet unknown, so additional measurements and modelling are needed. Moreover, when large amounts of liquid are added, two-phase flow calculations are necessary.

- The modelling of the stirrer is crude and requires measurements as input for the velocity field calculations. Computational Fluid Dynamics programs that enable the calculation of the flow around moving boundaries would be able to simulate the stirrer directly.

- Calculation of the deformation of drops with a viscosity that differs from that of the bulk is not possible yet. Visualisations show (see section 3.3) that low viscosity additions are deformed into sheets, whereas high viscosity additions form threads. A different model is required in each case.

6.4 Conclusion

The research project reported in this thesis has shown that, contrary to what was generally suspected to be the case in industrial blending operations, density differences strongly influence mixing times. Up to now long mixing times were mainly attributed to large viscosity differences. When liquid is added to the vessel near the stirrer, mixing times will be found to be relatively short. Unless buoyancy effects play a part, considerably longer mixing times do not occur.

The computational approach used in this study has made clear that it is possible to simulate adequately at least some aspects of the mixing process. All the signs are that in the foreseeable future CFD will allow more reliable predictions for the mixing performance in a given vessel even before the apparatus or a scale model is actually built. Numerical simulation will therefore become increasingly important to equipment designers. However, computational techniques will of necessity be complemented by experimental methods. A blend of the two methods must eventually lead to a clear understanding of the mixing process in all its aspects.
Nomenclature

(vectors are in bold typeface)

\[ a, b \quad \text{constants used to calculate } u^* \quad - \]
\[ Ar \quad \text{Archimedes number} \quad - \]
\[ B \quad \text{baffle width} \quad m \]
\[ C \quad \text{stirrer to bottom clearance} \quad m \]
\[ \langle C \rangle \quad \text{average marker concentration} \quad \text{kg/m}^3 \]
\[ C^* \quad \text{dimensionless concentration} \quad - \]
\[ C_e \quad \text{constant used to calculate } e \quad - \]
\[ C_f \quad \text{friction coefficient} \quad - \]
\[ C_t \quad \text{constant} \quad - \]
\[ C_{\mu} \quad \text{constant used to calculate } \tau \quad - \]
\[ c \quad \text{constant used to calculate } \Delta t \quad - \]
\[ D \quad \text{stirrer diameter} \quad m \]
\[ D \quad \text{diffusion coefficient} \quad \text{m}^2/\text{s} \]
\[ D_D \quad \text{central disc diameter} \quad m \]
\[ d \quad \text{disc thickness} \quad m \]
\[ d_0 \quad \text{initial diameter of cylinder} \quad m \]
\[ d_1 \quad \text{diameter of cylinder after } t_{\text{def}} \quad m \]
\[ E_m \quad \text{energy needed for the mixing process} \quad J \]
\[ e \quad \text{rate of extension} \quad \text{s}^{-1} \]
\[ Fo \quad \text{Fourier number} \quad - \]
\[ Fo_{\text{cr}} \quad \text{critical value of } Fo \quad - \]
\[ g \quad \text{gravitational acceleration} \quad \text{m/s}^2 \]
\[ H \quad \text{liquid height in the vessel} \quad m \]
\[ k \quad \text{turbulent kinetic energy per unit mass} \quad \text{J/kg} \]
\[ L \quad \text{blade length} \quad m \]
\[ l \quad \text{cell length} \quad m \]
\[ l_K \quad \text{Kolmogorov’s length scale of turbulence} \quad m \]
\[ N \quad \text{stirrer rotational speed} \quad \text{s}^{-1} \]
\[ N_l \quad \text{generated random number} \quad - \]
\[ N_t \quad \text{N where transition occurs} \quad \text{s}^{-1} \]
\[ n \quad \text{number of fluid elements or flow followers} \quad - \]
\[ P \quad \text{total power draw} \quad \text{W} \]
Nomenclature

\( P_{\text{probe}} \) \quad \text{fraction of particles passing the stirrer}

\( P_0 \) \quad \text{power number} \quad \frac{P}{\rho_0 N^3 D^5}

\( p \) \quad \text{probability of exceeding } \Delta

\( P_s \) \quad \text{simulated probability of surfacing}

\( R \) \quad = T/2, \text{ vessel radius} \quad \text{m}

\( Re \) \quad \text{Reynolds number} \quad \frac{\rho_0 N D^2}{\mu_0}

\( Re_d \) \quad \text{drop Reynolds number} \quad \frac{\rho_0 u_d d}{\mu_0}

\( Ri \) \quad \text{Richardson number} \quad \frac{\Delta p g H}{\rho_0 N^2 D^2}

\( r \) \quad \text{radial coordinate} \quad \text{m}

\( r^* \) \quad \text{dimensionless radius}

\( r \) \quad \text{randomly distributed random vector}

\( s \) \quad \text{distance between two points} \quad \text{m}

\( T \) \quad \text{vessel diameter} \quad \text{m}

\( T_b \) \quad \text{blade thickness} \quad \text{m}

\( t_c \) \quad \text{circulation time} \quad \text{s}

\( t_{\alpha} \) \quad \text{time after which } F_{\alpha} \text{ is reached} \quad \text{s}

\( t_{\text{def}} \) \quad \text{deformation time} \quad \text{s}

\( t_{\text{df}} \) \quad \text{diffusion time} \quad \text{s}

\( t_K \) \quad \text{Kolmogorov's time scale of turbulence} \quad \text{s}

\( t_m \) \quad \text{mixing time} \quad \text{s}

\( t_1, t_2 \) \quad \text{time between injection and first stirrer passage} \quad \text{s}

\( t_{p2} \) \quad \text{time between injection and second stirrer passage} \quad \text{s}

\( t_{\text{probe}} \) \quad \text{probe time in simulation} \quad \text{s}

\( t_{\text{tot}} \) \quad \text{total time for deformation and diffusion} \quad \text{s}

\( t_1, t_2 \) \quad \text{mixing times corresponding to } \Delta_1 \text{ and } \Delta_2 \quad \text{s}

\( t_{50\%} \) \quad \text{time needed for drop to reach 50\% of } u_{\text{buoy}} \quad \text{s}

\( \Delta t \) \quad \text{time step} \quad \text{s}

\( U_i \) \quad \text{uniform deviate}

\( u \) \quad \text{velocity} \quad \text{m/s}

\( u_{\text{buoy}}, u_{\text{buoy}} \) \quad \text{steady state relative velocity} \quad \text{m/s}

\( u_i(x_i) \) \quad \text{turbulent (rms) velocity at } x_i \quad \text{m/s}

\( u^* \) \quad \text{dimensionless velocity}

\( u(x_i) \) \quad \text{mean bulk velocity at } x_i \quad \text{m/s}
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>(V)</td>
<td>vessel volume</td>
<td>(m^3)</td>
</tr>
<tr>
<td>(V_a)</td>
<td>added liquid volume</td>
<td>(m^3)</td>
</tr>
<tr>
<td>(V_d)</td>
<td>drop volume</td>
<td>(m^3)</td>
</tr>
<tr>
<td>(W_b)</td>
<td>impeller blade width</td>
<td>m</td>
</tr>
<tr>
<td>(x)</td>
<td>normal random deviate</td>
<td>—</td>
</tr>
<tr>
<td>(x_i)</td>
<td>coordinate in the (i)-th direction</td>
<td>m</td>
</tr>
<tr>
<td>(x_i)</td>
<td>position at iteration (i)</td>
<td>m</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>deformation parameter</td>
<td>(s^{-1})</td>
</tr>
<tr>
<td>(\Delta)</td>
<td>mixedness criterion</td>
<td>—</td>
</tr>
<tr>
<td>(\Delta_1, \Delta_2)</td>
<td>values used for (\Delta)</td>
<td>—</td>
</tr>
<tr>
<td>(\gamma)</td>
<td>shear needed to cause break-up of drops</td>
<td>(s^{-1})</td>
</tr>
<tr>
<td>(\epsilon)</td>
<td>energy dissipation rate per unit mass</td>
<td>(W/kg)</td>
</tr>
<tr>
<td>(\mu)</td>
<td>viscosity</td>
<td>(Pa\cdot s)</td>
</tr>
<tr>
<td>(\mu^*)</td>
<td>(\text{def } \mu/\mu_0), viscosity ratio</td>
<td>—</td>
</tr>
<tr>
<td>(v)</td>
<td>kinematic viscosity</td>
<td>(m^2/s)</td>
</tr>
<tr>
<td>(\rho)</td>
<td>density</td>
<td>(kg/m^3)</td>
</tr>
<tr>
<td>(\Delta \rho)</td>
<td>(\text{def } \rho_a - \rho_0), density difference</td>
<td>(kg/m^3)</td>
</tr>
<tr>
<td>(\sigma)</td>
<td>standard deviation within series of measurements</td>
<td>—</td>
</tr>
<tr>
<td>(\tau)</td>
<td>maximum eddy lifetime</td>
<td>s</td>
</tr>
<tr>
<td>(\varphi)</td>
<td>angular coordinate</td>
<td>—</td>
</tr>
<tr>
<td>(\varphi_1, \varphi_2)</td>
<td>angular coordinate of stirrer plane crossing</td>
<td>—</td>
</tr>
</tbody>
</table>

**subscripts**

- \(a\) added liquid
- \(d\) drop
- \(z\) in the axial direction
- \(r\) in the radial direction
- \(\varphi\) in the angular or tangential direction
- \(0\) bulk

**abbreviations**

- A310 Lightnin A310 impeller
- CFD computational fluid dynamics
- CMC sodium carboxymethyl cellulose
- DT disc turbine
- LDV laser doppler velocimetry
- PBT pitched blade turbine
- PVP polyvinylpyrrolidone
References


Angst, W., Bourne, J.R. & Sharma, R.N. (1982); Mixing and fast chemical reaction—IV The dimensions of the reaction zone; Chemical Engineering Science, Vol. 37, No. 4, pp. 585-590


Beek, W.J. & Muttzall, K.M.K. (1975); "Transport phenomena"; John Wiley & Sons, Chichester

Bolzern, O. & Bourne, J.R. (1983); Mixing and fast chemical reaction—VI Extension of the reaction zone; Chemical Engineering Science, Vol. 38, No. 7, pp. 999-1003


createx (1990); "Fluent User’s Manual", Version 3.0, March 6; createx Incorporated, Hanover, NH

Gavlak, A.M. & Calabrese, R.V. (1989); Circulation time distribution in a turbinestirred tank; poster presentation at EF Mixing XII Conference, Potosi, Mo., USA

Grace, H.P. (1982); Dispersion phenomena in high viscosity immiscible fluid systems and application of static mixers as dispersion devices in such systems; Chemical Engineering Communications., Vol. 14, pp. 225-277


Ottino, J.M. (1989); "The kinematics of mixing: stretching, chaos, and transport"; Cambridge University Press

Ranade, V.V. & Joshi, J.B. (1989); Flow generated by pitched blade turbines I: measurements using laser doppler anemometer; *Chemical Engineering Communications*, Vol. 81, pp. 197-224

Ranade, V.V., Joshi, J.B. & Marathe, A.G. (1989); Flow generated by pitched blade turbines II: simulation using k-ε model; *Chemical Engineering Communications*, Vol. 81, pp. 225-248


Rielly, C.D. & Britter, R.E. (1985); Mixing times for passive tracers in stirred tanks; *5th European Conference on Mixing*, Würzburg, Germany, organised by VDI-Gesellschaft Verfahrenstechnik und Chemieingenieurwesen (GVC); pp. 365-375


Riet, K. van 't (1975); "Turbine agitator hydrodynamics and dispersion performance"; Ph.D. thesis, Delft University of Technology, The Netherlands

Smith, J.M. (1990); Industrial needs for mixing research; Transactions of the Institution of Chemical Engineers; Vol. 68, Part A, pp. 3-6
Smith, P.G., van de Ven, T.G. & Mason, S.G. (1981); The transient interfacial tension between two miscible fluids; Journal of Colloid and Interface Science, Vol. 80, No. 1, pp. 302-303
Tatterson, G.B. (1991); "Fluid mixing and gas dispersion in agitated tanks"; McGraw-Hill
Thýn, J., Novák, V. & Pock, P. (1976); Effect of the measured volume size on the homogenization time; The Chemical Engineering Journal, Vol. 12, pp. 211-217
Vusse, J.G. Van de (1955); Mixing by agitation of miscible liquids—Part I; Chemical Engineering Science, Vol. 4, pp. 178-200; Part II: pp. 209-220
Warmoeskerken, M.M.C.G. (1986); Gas-liquid dispersing characteristics of turbine agitators; Ph.D. thesis, Delft University of Technology, The Netherlands
Weetman, R.J. (1992); Lightnin, Rochester, New York, USA; personal communication
Wilmott, P. (1989); The stretching of a thin viscous inclusion and the drawing of glass sheets; Physics of Fluids A, Vol. 1, No. 7, pp. 1098-1103
Wu, H. & Patterson, G.K. (1989); Laser-Doppler measurements of turbulent-flow parameters in a stirred mixer; Chemical Engineering Science, Vol. 44, No. 10, pp. 2207-2221
Zlokarnik, M. (1967); Eignung von Rührern zum Homogenisieren von Flüssigkeitsgemischen; Chemie-Ingenieur-Technik, Vol. 39, No. 9/10, pp. 539-549
Curriculum Vitae

Ivo Bouwmans

24 oktober 1961 geboren te Rotterdam
1974 - 1980 gymnasium β, Emmauscollege, Rotterdam
1980 - 1986 studie Technische Natuurkunde, TU Delft
afstudeeronderwerp: ‘Het gedrag van sonische gasstralen in water’,
vakgroep Transportverschijnselen, sectie Fysische Technologie
(prof. J.M. Smith D.Sc.)
1983 lerarenopleiding nieuwe stijl, inclusief stage
1985 - 1986 studentlid van vakgroepsbestuur
‘Mengen van vloeistoffen met viscositeitss- en dichtheidsverschillen’,
vakgroep Transportverschijnselen, sectie Fysische Technologie
(prof.dr.ir. H.E.A. van den Akker)
1987 - 1988 docent van twee instructieseries en enkele colleges bij het college
Fysische Transportverschijnselen I
1987 - 1991 lid van bedrijfsbrandweer Kramers Laboratorium
1991 - ... toegevoegd onderzoeker bij Interduct—Delft University Clean
Technology Institute
1992 - ... calligraaf van promotie-bullen, TU Delft