



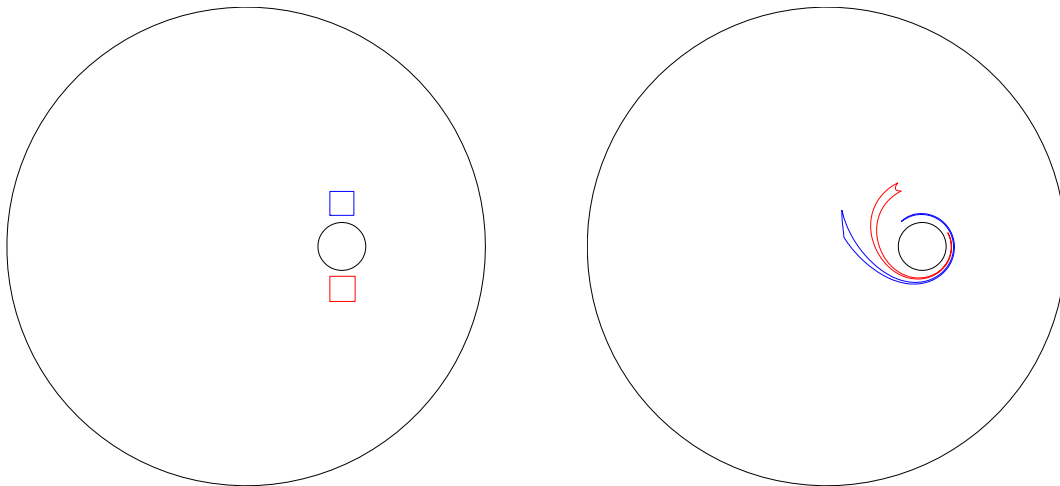
Kinematic evaluation of mixing in a two dimensional flow

Máté Tibor Szőke

Mechanical Engineering Modelling – Fluid and Solid Mechanics
1st year MSc student

Dr. Csaba Hős

Associate professor
Budapest University of Technology and Economics (BUTE)
Department of Hydrodynamic Systems



January 4, 2013

Contents

1	Introduction	3
1.1	Motivation	3
1.2	Overview	3
1.3	Literature review	4
2	The CFD calculations	6
2.1	Geometry creation and discretization	6
2.2	Boundary conditions and solver set-up	7
2.3	Mesh convergence study	7
2.4	Effect of turbulence models	8
3	Techniques of evaluating stirring ability	12
3.1	Tracing fluid packages	12
3.2	Statistical approach	13
3.3	Principal deformations	15
4	Results	16
4.1	The flow fields to be analysed	16
4.2	Tracing fluid packages	16
4.3	Statistical approach	20
4.4	Principal deformations	24
5	Summary	26

1 Introduction

1.1 Motivation

The mixing of two or more fluids is a common industrial task. The goal of sizing the mixer is to achieve a homogeneous mixture within reasonable time, by consuming acceptable amount of energy. When analysing different mixer geometries or flow conditions, one encounters the problem that the “goodness” of mixing is highly challenging to quantify, especially in the case of real-life (complex) geometries and flow fields. There is no ultimate, widely accepted measure to evaluate the mixing ability.

The goal of this study is the investigation of the mixing ability of a cylindrical flow field in which there is an eccentrically placed rotating mixer element. More precisely, *we intend to evaluate three techniques of measuring mixing ability from the engineering point of view*. These three techniques are

- a self-developed method computing the deformation of fluid “packages”,
- a statistical approach monitoring the standard deviation of the concentration of marker particles and
- a third approach focusing on the local stretching properties based on the velocity gradient tensor.

All these methods require the velocity field a priori, which was calculated by CFD simulations. Further calculations were carried out in MATLAB .

1.2 Overview

During the design of mixing devices the designer have to answer many questions. What would be the optimum size of the tank? What is the most efficient size, location, orientation and revolution speed of the mixing element? What will be the operation time? These questions are hard to decide for the first time, however many of them must be answered during a design process.

There are some available literature of mixing devices in which one can find recommendations about the main sizes of such instruments, see e.g. [11]. It is also often described how to choose the appropriate motor to make the impeller work. Unfortunately there is a limited description about how much time is it going to take to mix the inserted materials in the vessel.

One can find further descriptions in the literature of topologies about how materials can be deformed, stirred, stretched or mixed, see e.g. [1]. For example a very famous example from chaos theory is the so-called horseshoe map [5] in which a racecourse shaped fluid element is firstly stretched, then secondly folded into the shape of a horseshoe (see Figure 3). This theory can describe the “life” of a fluid parcel around a stirrer in such mixers like ours.

In this study, a simplified cylindrical geometry was investigated, in which we assumed a two-dimensional flow. The rotational mixing element had a cylindrical shape as well, and it was placed eccentrically in the cylinder. We calculated the velocity field with the help of a CFD software. The effect of the spatial resolution and the turbulence modelling was investigated also.

This report is organized as follows. After giving a literature overview in Section 1.3, the next topic is the detailed description of the CFD simulations (Section 2). The methods which were

used to evaluate the mixing ability of the flow field are reported in Section 3. Then, in Section 4 the results were plotted and evaluated.

1.3 Literature review

Topology is the area of mathematics that deals with the continuous deformation of shapes. In this field one can find descriptions about mixing and stirring materials, e.g. [1]. This paper introduces the basic set-ups (protocols) and descriptions of the so called generic “batch” stirring device, which consists of a vessel and stirrer(s) (see Figure 1). The basic idea is to place k number of stirrers into the media and rotate them, change the direction of their rotation and move the stirrers in the fluid.

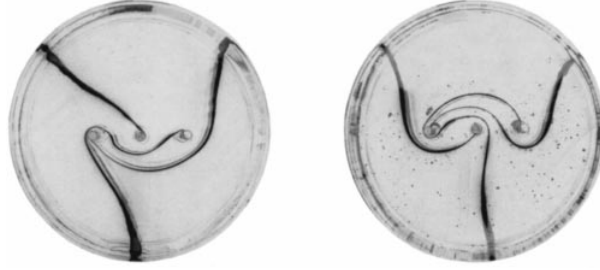


Figure 1: A generic “batch” stirrer with three embedded stirrers – picture was taken from [1]

A detailed and highly cited bibliography within this topic is J. M. Ottino’s book [9], which investigates the behaviour and properties of mixing. The basic idea is to place an elemental fluid line into the flow ($d\mathbf{X}$) and apply the motion ($\Phi(\mathbf{X}, t)$) on this element, which yields to a distorted $d\mathbf{x}$ ($d\mathbf{x} = \Phi(d\mathbf{X}, t)$) element line. Between these states the stretch ratio is defined as follows

$$\lambda = \lim_{|d\mathbf{X}| \rightarrow 0} \frac{|d\mathbf{x}|}{|d\mathbf{X}|} = \lim_{|d\mathbf{X}| \rightarrow 0} \frac{|\Phi(d\mathbf{X}, t)|}{|d\mathbf{X}|}. \quad (1)$$

This value stands for characterising the mixing and stirring ability of the flow. Ottino states that in a well mixing flow field the efficiency of mixing does not to converge to zero in time, which is defined as

$$\eta = \frac{d}{dt} \ln \frac{|d\mathbf{x}|}{|d\mathbf{X}|}. \quad (2)$$

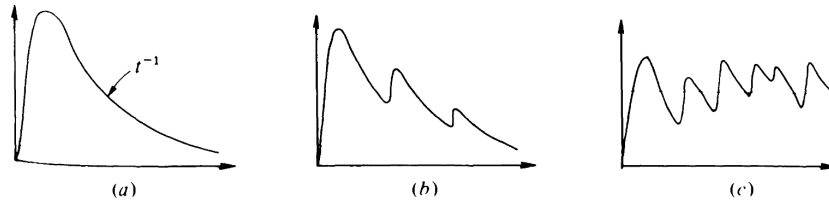


Figure 2: Typical behaviours of mixing efficiency – picture was taken from [9]

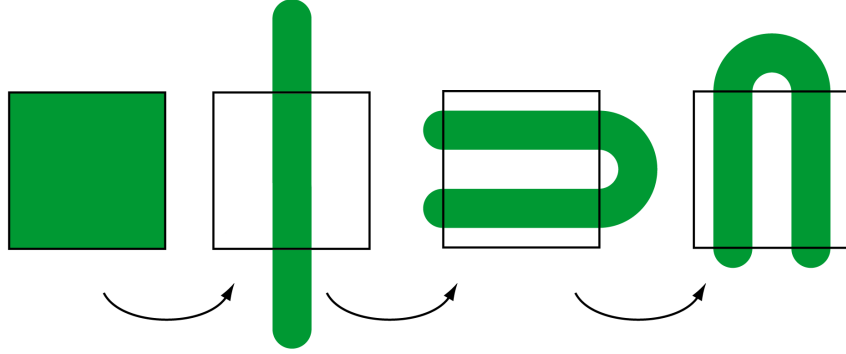


Figure 3: The horseshoe mapping [5]

Ottino distinguishes three different types of mixing efficiency behaviour, which can be seen on Figure 2. The first one marked with (a) is the worst mixing case, where η tends to zero, (b) is a flow with partial restoration, meaning better mixing and the (c) case is the best mixing flow, which has both stretching and reorientation. The importance of reorientation is that it – roughly speaking – “restarts” the stretching process at $t = 0$, where the stretching is the most intensive. Moreover, the continuous reorientation introduces a horseshoe-like map [5], which is a basic example of the chaos theorem, in which a fluid element is stretched (see Figure 3), folded into U shape, and then reorientated (rotated) – these sequences are executed periodically in time. The basic idea of this mapping is in parallel with the same idea written by Ottino:

$$\boxed{\text{good mixing} = \text{stirring} + \text{reorientation}.}$$

In order to reach a non-zero value in η , the increment of the length of the elemental line needs to be exponential. Suppose that the stretching is polynomial in time, i.e. $|\mathrm{d}\mathbf{x}|/|\mathrm{d}\mathbf{X}| = At^n$ where the initial length is stretched in time t . Then, we have

$$\eta = \frac{\mathrm{d}}{\mathrm{d}t} \ln(At^n) = \frac{n}{t}, \quad (3)$$

which tends to zero if time tends to infinity, which implies a bad quality of mixing. But in the case of $|\mathrm{d}\mathbf{x}|/|\mathrm{d}\mathbf{X}| = e^{At}$ the expression gives a good mixer flow:

$$\eta = \frac{\mathrm{d}}{\mathrm{d}t} \ln(e^{At}) = A. \quad (4)$$

In this case, the mixing efficiency tends to A , which is a constant value, therefore in the second case the flow mixes better than in the former one.

The locally defined velocity gradient matrix [6] is what includes both *stretching* and *rotating* property of the flow, the symmetrical part of which is the so called rate of strain tensor. This tensor acts on fluid particles so that it generates the length changes. The eigenvalues of this matrix describe the flow properties locally, therefore by knowing these values one can investigate a streamline and check that what kind of regions of such eigenvalues does the streamline pass. With these values the “history” of a particle can be predicted.

These papers motivated us to start with a relatively simple geometry. In what follows, we study the mixing in a cylindrical tank with an eccentrically located circular mixing element, as shown on Figure 4.

2 The CFD calculations

2.1 Geometry creation and discretization

While creating the geometry, the main goal was the representation of the mixing volume of the mixer in such a simplified way that allows simple CFD computations yet gives realistic results¹. It was also important to keep the computational efforts within reasonable limits, especially given the fact that the computation of the flow field is not the ultimate goal of this study but only the input data of the main computations. Based on these restrictions a two-dimensional cylindrical mixing area were chosen – this represents the perpendicular cross section of mixing vessel. Within this domain a simplified stirrer was placed eccentrically, which was chosen to be cylindrical. The created geometry (and mesh) can be seen on Figure 4(a) (and Figure 4(b)).

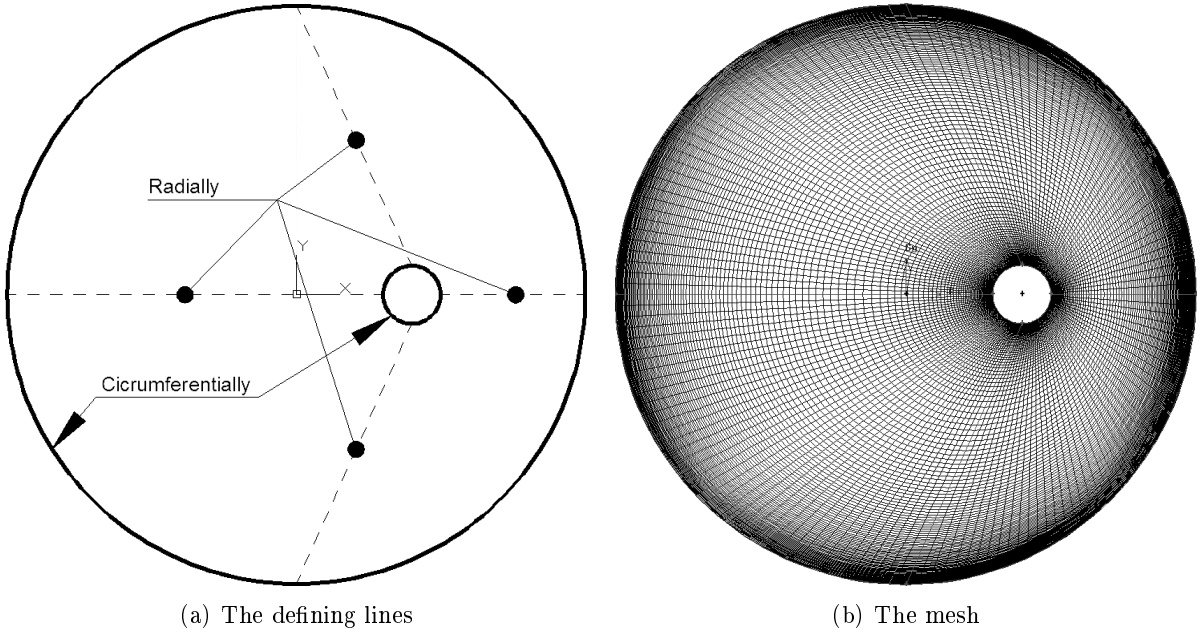


Figure 4: Mesh creation

The dimensions of the geometry are the followings: the radius of the mixer is 1 [m], the radius of the stirrer within the mixer is 0.1 [m], and it has an eccentricity of 0.4 [m] along the x axis.

The geometry and the mesh for the simulations were created in ANSYS Gambit. Boundary layer meshes were generated on the wall of the mixing element and on the wall of the vessel. The properties of the boundary layer mesh can be found in Table 1. The represented values were defined “experimentally”: they were changed until the desired y^+ value [6] was reached – for the “practical” case – in the simulations. The inflation ratio away from the walls is less then 10 %. The number of elements in the radial and tangential directions were systematically increased – see Table 1 and the grid independence study in Section 2.3. The mesh quality was inspected in ANSYS ICEM due to ANSYS Gambit is not capable of exporting the mesh directly for ANSYS

¹Several attempts were made to find a closed-form synthetic flow field but it was found that these oversimplified solutions are not realistic.

<i>Property</i>	<i>“Coarse”</i>	<i>“Practical”</i>	<i>“Dense”</i>
Total element number	56 320	112 000	448 000
Height of the 1 st element at wall of mixer ($\cdot 10^{-7}$ [m])	513	265	133
Height of the 1 st element at wall of vessel ($\cdot 10^{-5}$ [m])	130	66	33
Element number along the circumference of the circles	160	320	640
Element number between the mixer and outer wall	175	350	700
Worst determinant [3] value ($\cdot 10^4$)	9575	9786	9695

Table 1: Mesh properties

CFX. The worst determinant [3, p. 46.] value of the mesh was 0.968 which is a highly above the usual minimum requirements.

2.2 Boundary conditions and solver set-up

The outer wall of the mixer was chosen to be a standing wall. The wall of the mixing element was a rotational wall: it rotates about its own axis ($x = 0.4$ [m] $y = 0$ [m]) with a constant revolution number. The remaining surfaces (being normal to z direction) were set to symmetries – this resulted a two-dimensional flow in the CFX simulations.

Before starting the iterations some more set-ups had to be applied. During the simulations the $k-\omega$ SST (Shear Stress Transport, see [2] for details) turbulence model was used. It is useful to monitor the results at certain place in the domain, while the iterations are going on, therefore at the point $[x = 0.39, y = 0, z = 0]$ [m] the velocity and the pressure was checked. Each simulations run till the point when each residual reached its own minimum and the velocity in the monitored point converged. Convergence criteria were set to less then 10^{-6} . Upwind advection scheme was used.

The simulations were run on the computers of the Department of Hydrodynamic Systems. The environment was ANSYS CFX. Double precision was set up in the solver in order to minimize the rounding errors.

2.3 Mesh convergence study

To make sure that the results given by the solver are acceptable it was reasonable to carry out a mesh convergence study. This meant that a lower (“coarse”) and a higher (“dense”) spatial resolution mesh was created. The size of the elements was decreased and increased so that the element number along each line – along the circles and along x and y axis – were doubled and halved (see Figure 4(a)). In line with this the height of the first element was also changed: halved and doubled as well (oppositely). The calculated velocity distribution along the x (Figure 5) and y (Figure 6) axis was exported and plotted. Along with this, one can see the errors of the velocities (calculated according to (5)) along the x and y axes and the error distribution also, which was defined as

$$\varepsilon = \frac{v_f - v_i}{v_c} \cdot 100 [\%], \quad (5)$$

where v_f is the velocity calculated with the “fine mesh”, v_i is the velocity calculated with the investigated mesh (“practical” or “coarse”) and v_c is the circumferential velocity of the stirrer. After inspecting these results one can see that the so called “practical” – which attributes is described in Section 2.1 – mesh gives acceptable results. Therefore to carry out more calculations this “practical” mesh is reasonable to use.

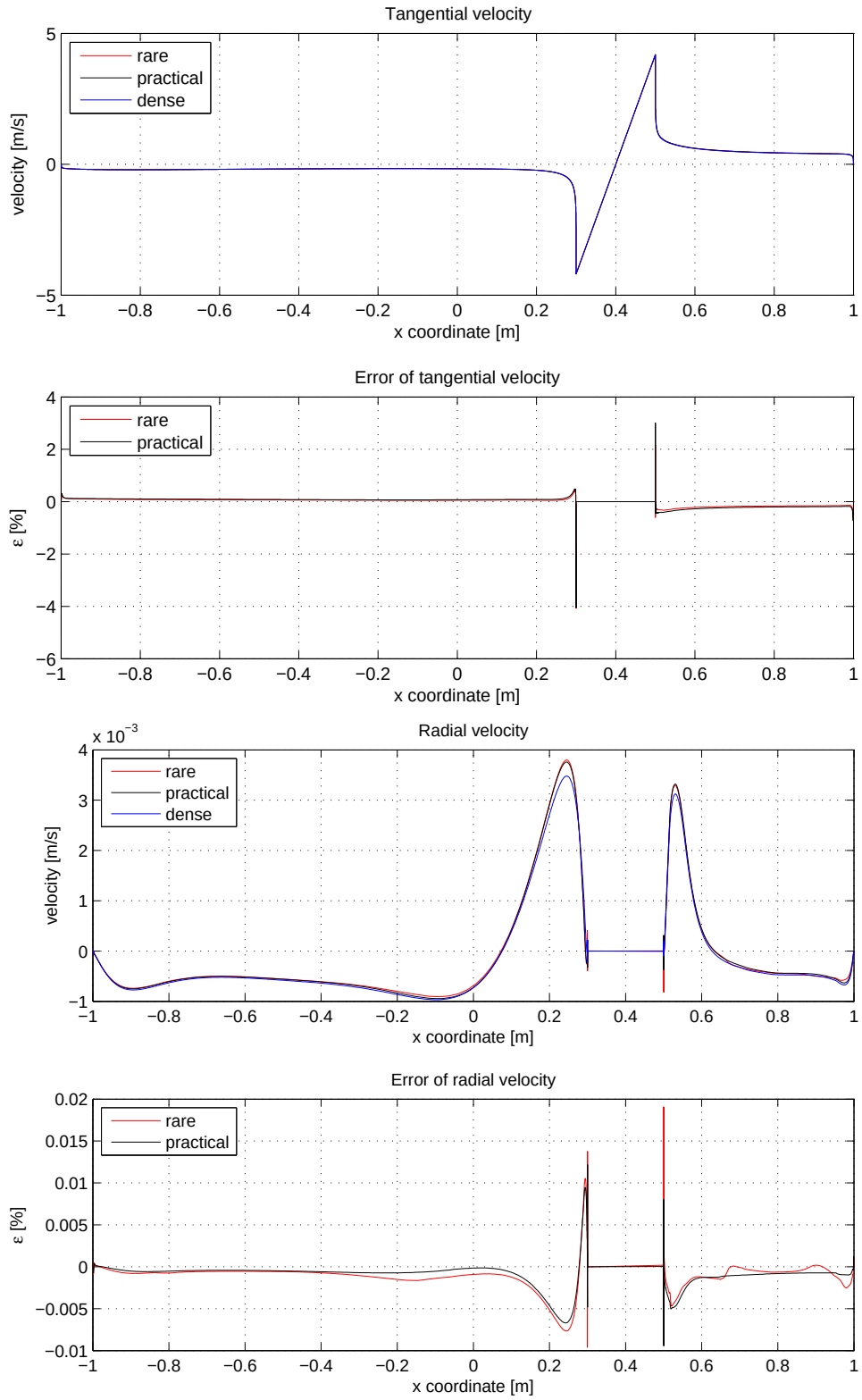
2.4 Effect of turbulence models

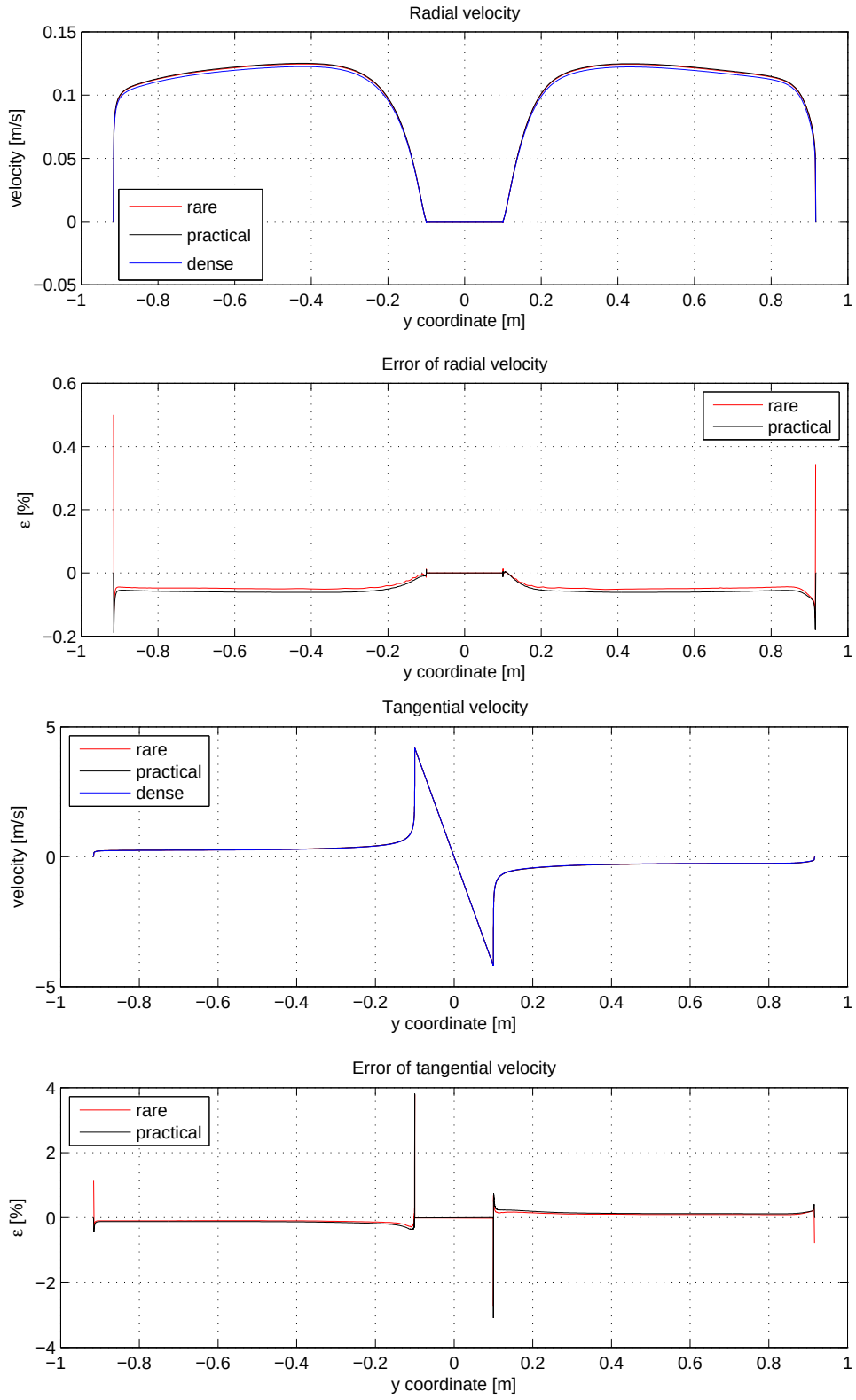
In the previous calculations the k- ω SST turbulence model was the responsible RANS² model. In what follows, the effect of different turbulence models (see [2]) are to be investigated, which are

- k- ε ,
- k- ω and
- k- ω SST.

The different results are plotted along $x = 0.4 [m]$ and $y = 0 [m]$ on Figure 7. The k- ω SST model differs in the radial case from the other two models, however that model seems to give – from engineering point of view – the best solution. In the axial case there is not much difference between the models. Therefore in the MATLAB simulations the results given by the k- ω SST model is to be used.

²Reynolds-averaged Navier-Stokes

Figure 5: Mesh convergence study: the velocity and error distribution along the x axis

Figure 6: Mesh convergence study: the velocity and error distribution along the y axis

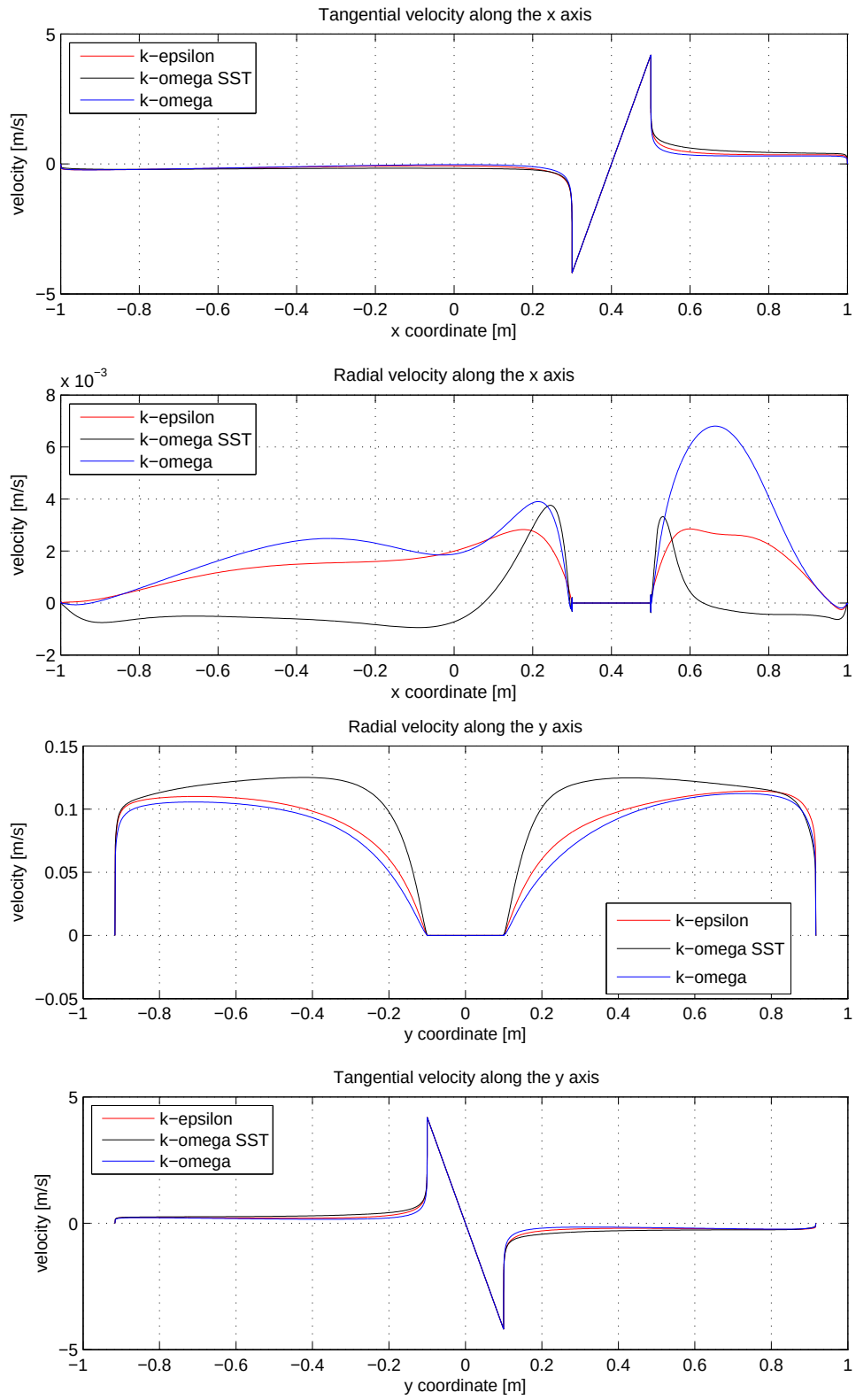


Figure 7: The velocity distributions with different turbulence models

3 Techniques of evaluating stirring ability

3.1 Tracing fluid packages

After calculating the velocity field in CFX it was imported into MATLAB for further investigations. In MATLAB the following differential equation was solved numerically by the built-in `ode45` solver [7]:

$$\begin{bmatrix} \dot{x}(t) \\ \dot{y}(t) \end{bmatrix} = \begin{bmatrix} v_x(x, y) \\ v_y(x, y) \end{bmatrix}. \quad (6)$$

In (6) on the left hand side $\dot{x}(t)$ and $\dot{y}(t)$ are the time derivatives of the coordinates, on the right hand side $v_x(x, y)$ and $v_y(x, y)$ are the velocity components. The functions $x(t)$ and $y(t)$ are responsible to describe the path of an elemental fluid particle.

We have placed two fluid packages into the flow field and followed their “history”. The packages were rectangular at the time instant $t = 0$ [sec], each had N elements along their circumference. This also meant that there were Δs distance between each node. A package can be seen on the left hand side of Figure 8. Due to the mixing and stirring property of the velocity field, our package changed its shape in time. The code paid attention to the Δs distance between the nodes after each time step and if the distance increased more than a pre-defined threshold (Δs_{max}) than the program inserted additional nodes along the stretched element. This process is marked by green on Figure 8, furthermore in the case when a point got closer to an other one than an also pre-defined value (Δs_{min}) than MATLAB deleted that point from the package – see the red coloured dot on the right hand side of Figure 8. This adaptation process helped us conserving the area of the package and the problem remained approachable by assuming local changes.

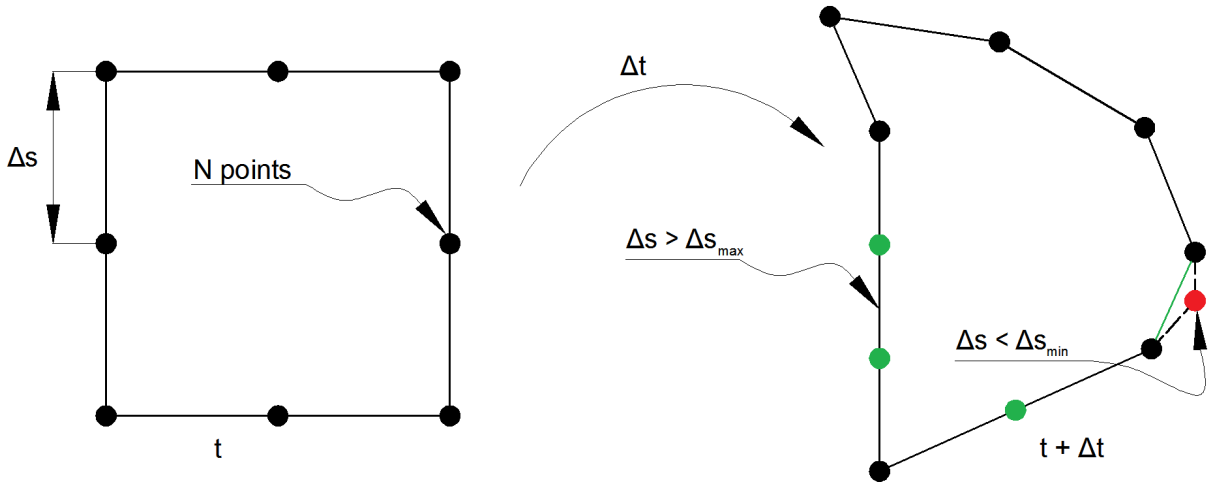


Figure 8: The point adaptation process

An important result of this simulation is the “history” of the perimeter ratio, which was the ratio of the actual ($P(t)$) and the initial perimeter P_0 , i.e. $P(t)/P_0$.

To monitor the accuracy of the simulation, we continuously monitored the actual area of the package, which is supposed to be constant (the flow is 2D and incompressible). We allowed

10 % of error in this value during these simulations and once this error bound was reached, the simulation was terminated.

For evaluating the “mixing” of the flow field, we used the following two indicators based on the perimeter.

- On one hand, we calculated the relative perimeter $P(t)/P_0$. This essentially measures the rate of stretching.
- On the second hand, based on Ottino’s work [9], we define

$$\eta = \frac{d}{dt} \ln \frac{P(t)}{P_0}, \quad (7)$$

which expression was based on (2) in which we changed the $|d\mathbf{x}|/|d\mathbf{X}|$ expression to $P(t)/P_0$, which is based on a chain of element lines. η was computed with centre difference scheme in time [4]. For the underlying considerations, we refer to Section 1.3.

3.2 Statistical approach

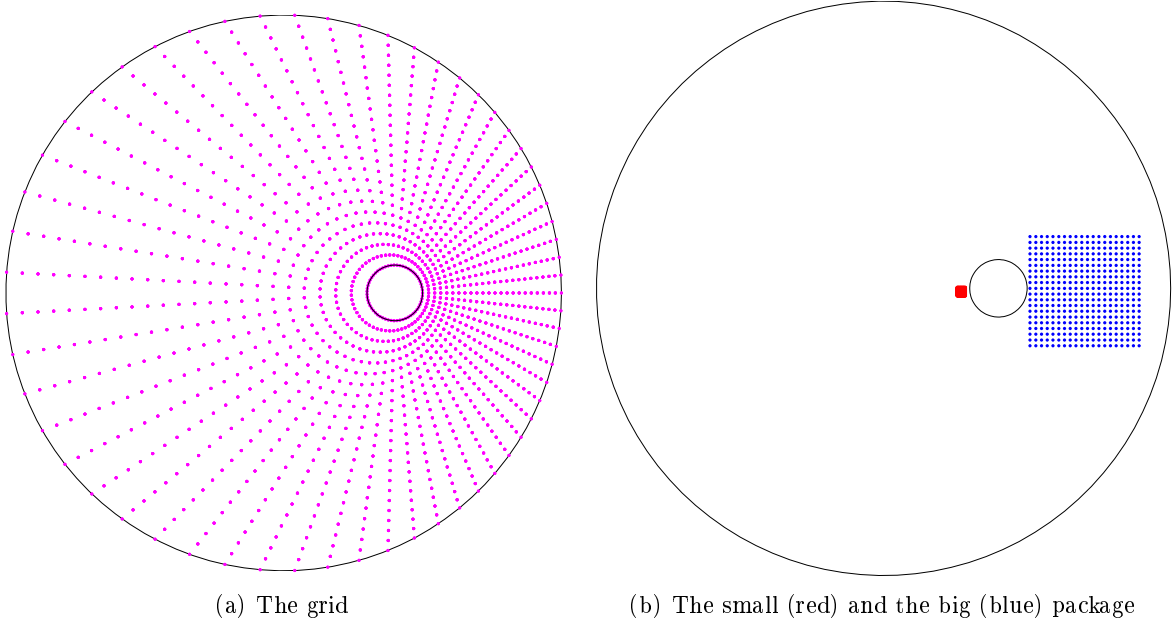


Figure 9: The grid (left) and the packages (right)

The mixing efficiency was investigated via statistical approach: the standard deviation of traced points was monitored. The flow field was split up into N_{rad} parts along radial direction and N_{tan} parts along tangential direction, this resulted $N_{rad} \cdot N_{tan} = N_c$ number of cells, the corner points of which are marked by dots on Figure 9(a). Each cell had a square shape. In the beginning of these simulations an also square shaped package with $M^2 = N_e$ number of elements

was placed into the mixer (see two of such packages on Figure 9(b)). The mean concentration was constant, which was defined as

$$\bar{c} = \sum_{i=1}^N \frac{c_i}{N}. \quad (8)$$

In this equation $c_i = N_i/1 = N_i$ is the concentration in the i^{th} cell, which is equal to the number of elements – in the followings N_i is used instead of c_i . The standard deviation was defined as

$$s^* = \sqrt{\frac{1}{N-1} (\bar{c} - c_i)^2}. \quad (9)$$

The best mixing is reached, when we spread all the elements as “well” as possible: the pigeon-hole principle [10] can help us to determine the best reachable standard deviation. In our case, *we had more elements than cells*, therefore we need to put more elements into one cell. To determine the best s^* let’s split up the elements into two parts:

$$\frac{N_e}{N_c} = \frac{(N_e - N_r) + N_r}{N_c} = \frac{K \cdot N_c + N_r}{N_c} = \underbrace{K}_1 + \underbrace{\frac{N_r}{N_c}}_2. \quad (10)$$

This means that we can place K pieces of elements – marked with “1” – into every cell and a number of N_r – marked with “2” – remaining elements should be distributed properly. Therefore we are meant to place the elements in order to reach our goal into the cells as followings:

$$\underbrace{K \cdot (N_c - N_r)}_{\text{cells with K pcs of elements;}} + \underbrace{N_r \cdot (K + 1)}_{\text{cells with K+1 elements}}. \quad (11)$$

With the help of this, the best available standard deviation is the following:

$$s_\infty^* = \sqrt{\frac{1}{N_c - 1} \left[(N_c - N_r) \cdot (\bar{c} - K)^2 + N_r \cdot (\bar{c} - (K + 1))^2 \right]}. \quad (12)$$

This number is a theoretical limit, which can not be reached within a finite time but we can define a relative residual deviation (RRD) based on the reached s^* in order to grade our mixer:

$$RRD = \left| \frac{s_\infty^* - s^*}{s_\infty^*} \right|. \quad (13)$$

We have placed two kind of element packages into the mixer: a “small” package, and a “big” package, see Figure 9(b). The “small” means that in the initial state the package was able to fit into a few cells, which condition was not satisfied in the second case, because that occupied many cells.

3.3 Principal deformations

The velocity gradients were exported from the CFD solver, and we used them to create the so called $\underline{\underline{D}}$ velocity gradient matrix [6, pp. 78.]. This meant that at each node of the mesh – used by the CFD solver – the following matrix was generated:

$$\underline{\underline{D}} = \begin{bmatrix} \frac{\partial v_x}{\partial x} & \frac{\partial v_x}{\partial y} \\ \frac{\partial v_y}{\partial x} & \frac{\partial v_y}{\partial y} \end{bmatrix}. \quad (14)$$

We have calculated the symmetric part of $\underline{\underline{D}}$ in the following form:

$$\underline{\underline{A}}_{sym} = \frac{1}{2} (\underline{\underline{D}} + \underline{\underline{D}}^T). \quad (15)$$

$\underline{\underline{A}}_{sym}$ is the so called rate of strain tensor [6, pp. 78–80.], which stands for the evaluation of angle and length changes of fluid elements in the flow field. The next step was the calculation of the eigenvalues (κ_1 and κ_2) of this matrix, which gave us the principal stretches. We would like to take a remark here that the equation $\text{trace}(\underline{\underline{A}}_{sym}) = 0$ gives us the continuity equation:

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0. \quad (16)$$

With the help of the bigger eigenvalues of these matrices we could generate a contour plot of the eigenvalue distribution in the flow field, which described whether where did the velocity field stretched the fluid elements the most. This helped us to evaluate the mixing from qualitative point of view as well.

4 Results

4.1 The flow fields to be analysed

In what follows, we compare the mixing properties of three different angular velocities of the stirrer: 100, 400 and 1600 rpm. As one can see, we quadruplicated the angular velocity twice. The first value is still quite low, mainly because in this case the mixing element rotates counter-clockwise about its own axis approx. 1.67 times in a second, while in the last case the rotation is so high that this shaft rotates approx. 26.67 times about its own axis in a second.

We shall evaluate these fields with the help of the techniques described in Section 3.

During the evaluation of the results we tried to focus on the mixing properties of the chosen geometry and we highlighted the similarities and the differences between the results and we have compared them with the expectations.

4.2 Tracing fluid packages

Two packages were placed symmetrically into the flow field, this can be seen on Figure 10(a). The first package (blue) was placed over the stirrer (inner black circle), and the second one (red) was placed under it, this means that the two packages were placed symmetrically. On Figure 10(b) the deformed packages (after 4 sec of simulation) can be seen for the 400 rpm case.

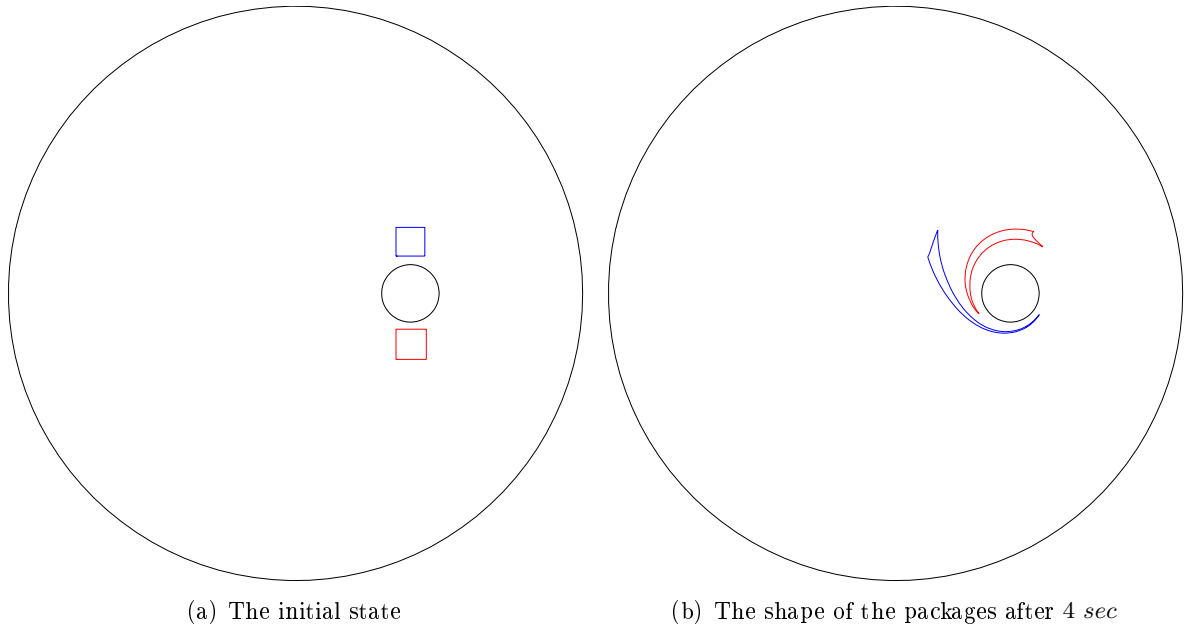


Figure 10: The two packages in the beginning and after 4 sec (400 rpm case)

The time step for the first two cases (100 rpm and 400 rpm) was 0.01 sec, for the third case – due to the very high velocities – Δt was 0.005 sec. The element number along one side of the rectangle was the same in the first two cases: 20 elements, while in the third case it was 100 elements per side.

Table 2 shows the simulated time for the different simulation cases and the required computation time. This data shows that the third case enormously increased the computation time compared to the first and second case.

<i>Case</i>	<i>Simulated time</i>	<i>Computation time</i>
100 rpm	15.43 <i>sec</i>	8.5 <i>hrs</i>
400 rpm	13.48 <i>sec</i>	22.0 <i>hrs</i>
1600 rpm	1.64 <i>sec</i>	44.5 <i>hrs</i>

Table 2: Properties of the tracing simulations

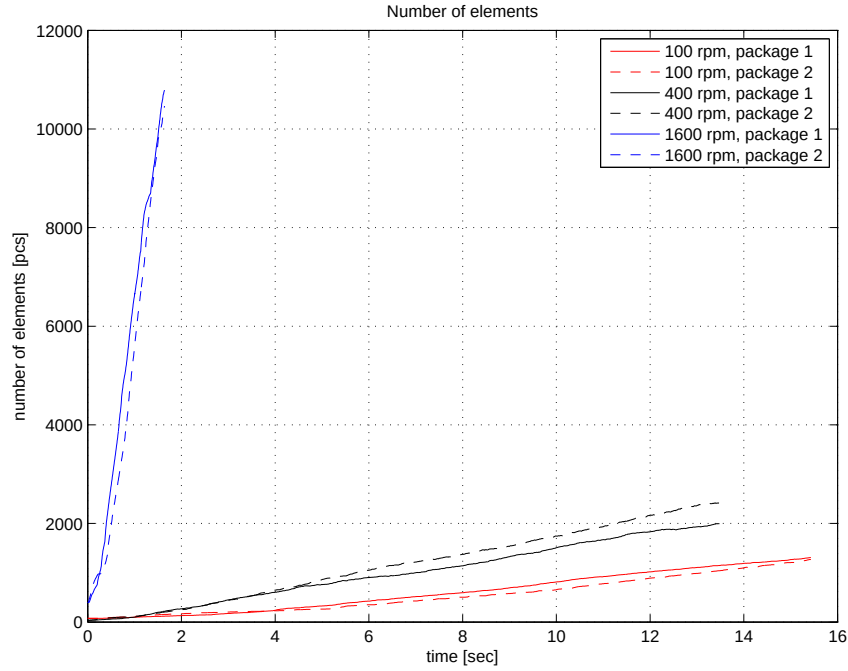


Figure 11: The number of elements along the perimeters of the packages in time

It can be seen on Figure 11 that despite of the higher initial resolution along the perimeter, we have experienced a very rapid increase in the necessary number of elements in the 1600 rpm case. In contrast, the resolution used in the other two simulations was enough to serve the requirements, which meant that the simulations could have been run longer. We have also implemented a $\pm 10\%$ of error tolerance in the perimeter ratio: once this was reached during the simulation, it was stopped automatically. This can be seen on the videos – which were attached to this document – showing the whole adaptive simulations that they end when the $\pm 10\%$ error is reached.

Figure 12 shows that although using a much finer time and spatial resolution in the third simulation it could run much shorter time, than the other two until it had step out of the error tolerance region. The 400 rpm case was simulated much longer time in order to inspect the

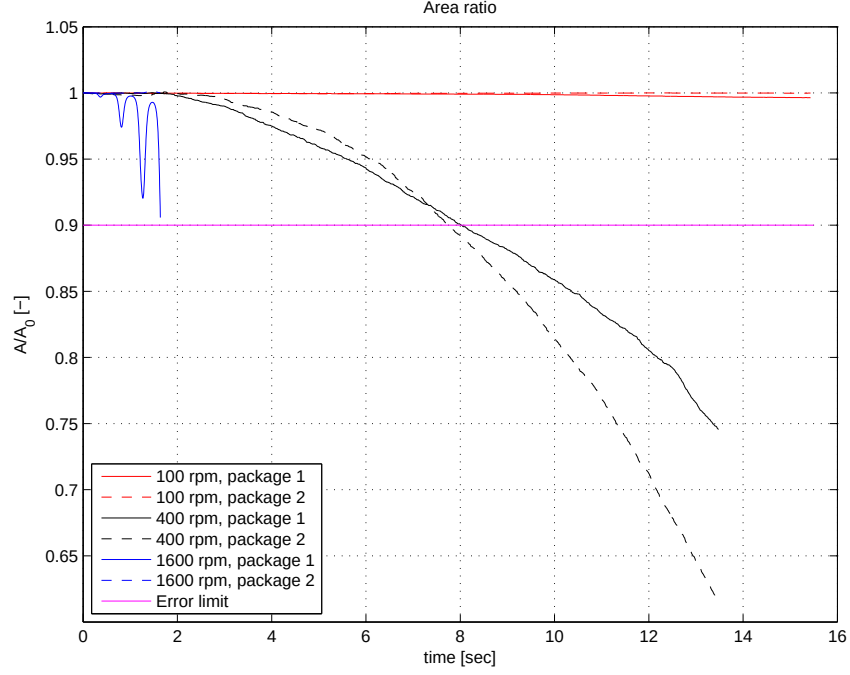


Figure 12: The area ratios during the simulations

“history” of the perimeter ratio deeper. The error tolerance was marked with a line at the 90 % of error on Figure 12. It can be also seen on Figure 12 that for the 100 rpm case the error did not increase as intensively than in the second or third case, which means that the lower the speed of revolution, the less the material is stirred – which we discovered as a cause of error in our simulations.

On Figure 13 one can see the values of $P(t)/P_0$. The third case reached the biggest steepness (most intensive stretch), which meets our expectations. For the medium and low rpm cases the curves are quite similar to each other, but the 400 rpm case causes higher stretch in both packages at every time instant. Our investigations showed that the perimeter ratio does not tends to a constant value, this can be seen on Figure 13.

On Figure 14 we can see the mixing efficiency (η , (7)), which tends to zero because it has a $1/x$ shape in every case. According to the bibliography [9], this implements a less increment in $P(t)/P_0$ than exponential, which corresponds to Figure 13. We can also see a wavy behaviour of these curves, which shows us the distorted nature of the flow field along the perimeter of the stirrer, furthermore it also shows that with how much speed does the mixing element rotates.

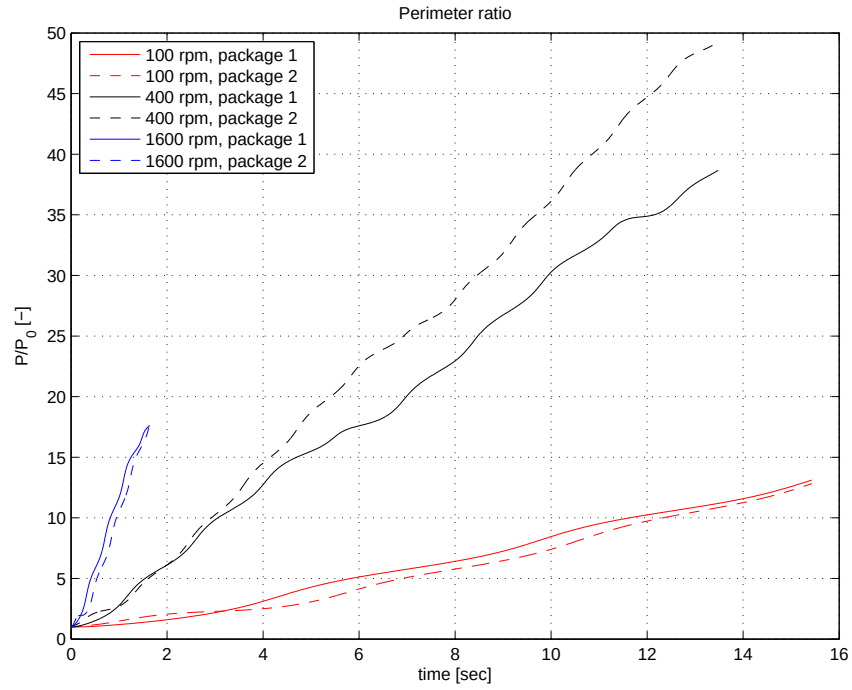


Figure 13: The perimeter ratios

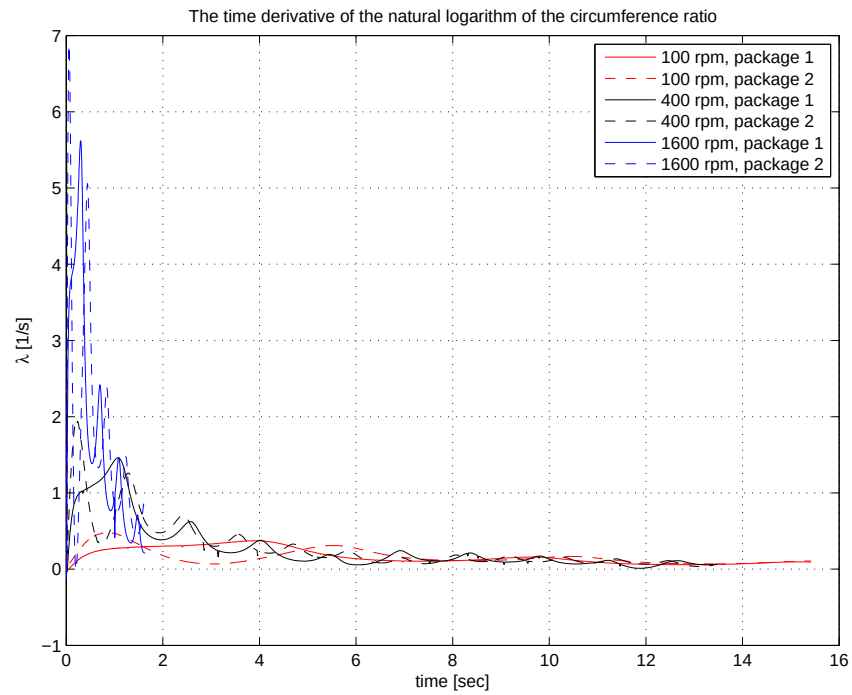


Figure 14: The time derivative of the natural logarithm of the area ratios

4.3 Statistical approach

Two different packages were introduced into the flow. On Figure 15(a) the “small” package can be found, while on Figure 15(b) the “big” package can be seen.

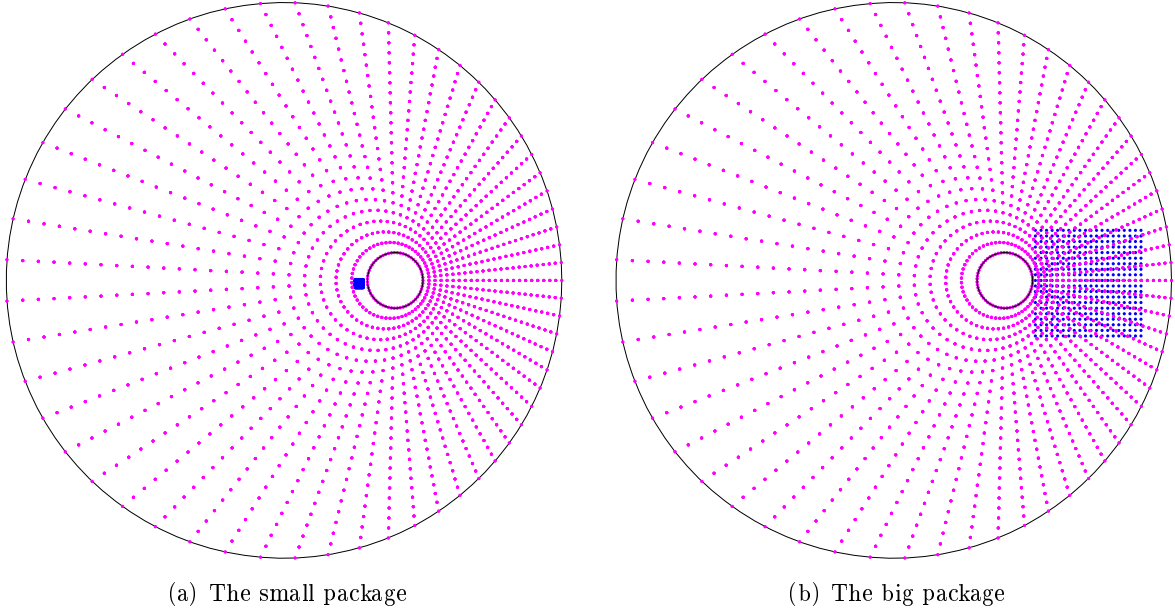


Figure 15: The beginning of the statistical simulations (with the grid)

The “small” package means 30 by 30 ie. 900 elements, while the “big” package means 20 by 20 ie. 400 elements. The time step was the same in every simulations as before: 0.01 *sec*. We attached the videos showing these simulations. Each video shows a simulated time of 25 *sec*. The theoretical limit of standard deviation (s_{∞}^* , (12)) for the first case is 0.3147, and for the second case it is 0.5007. The reached standard deviation (s^* , (9)), and the relative residual deviation (RRD , (13)) can be seen in Table 3.

<i>Simulation</i>	<i>Package type</i>	s^*	$\frac{pcs}{\sqrt{cell^3}}$	$RRD [-]$
100 rpm	small	3.219		5.430
	big	1.482		3.709
400 rpm	small	3.290		5.571
	big	1.139		2.618
1600 rpm	small	3.400		5.791
	big	0.723		1.296

Table 3: The reached s^* and relative residual deviations

As it was expected the most intensive mixer set-up reached the lowest average standard deviation in the same time frame. The relative residual deviation is in correlation with s^* , the best RRD is reached by the 1600 rpm case also. Figures 16 shows the shape of the packages

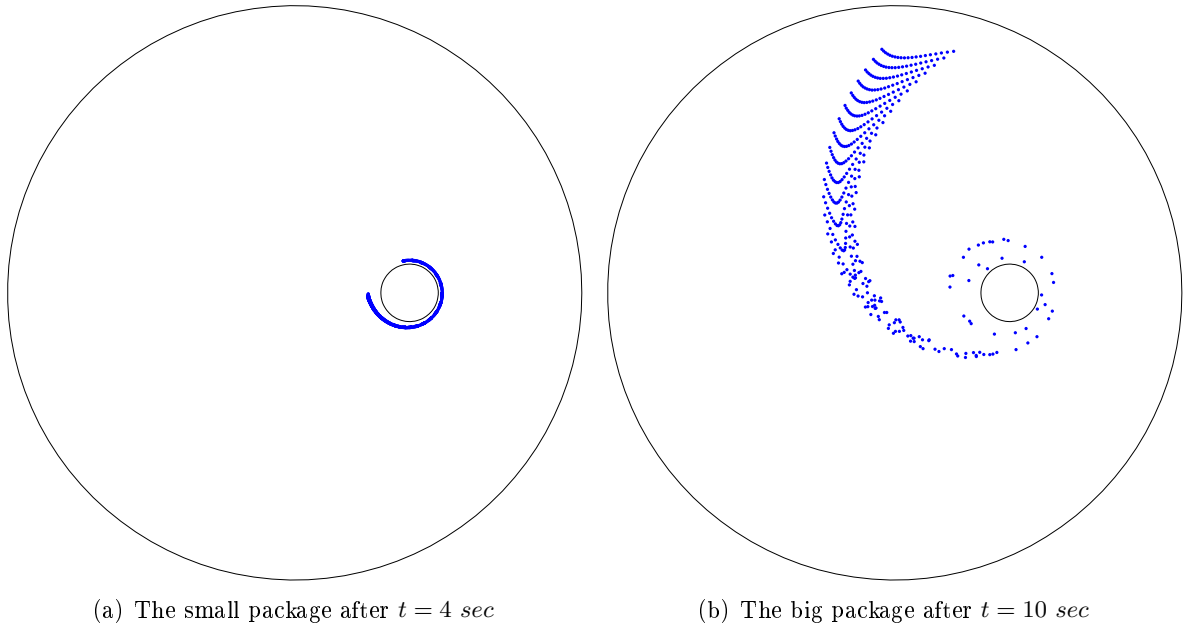


Figure 16: The statistical simulations for the 1600 rpm case after different times (without the grid)

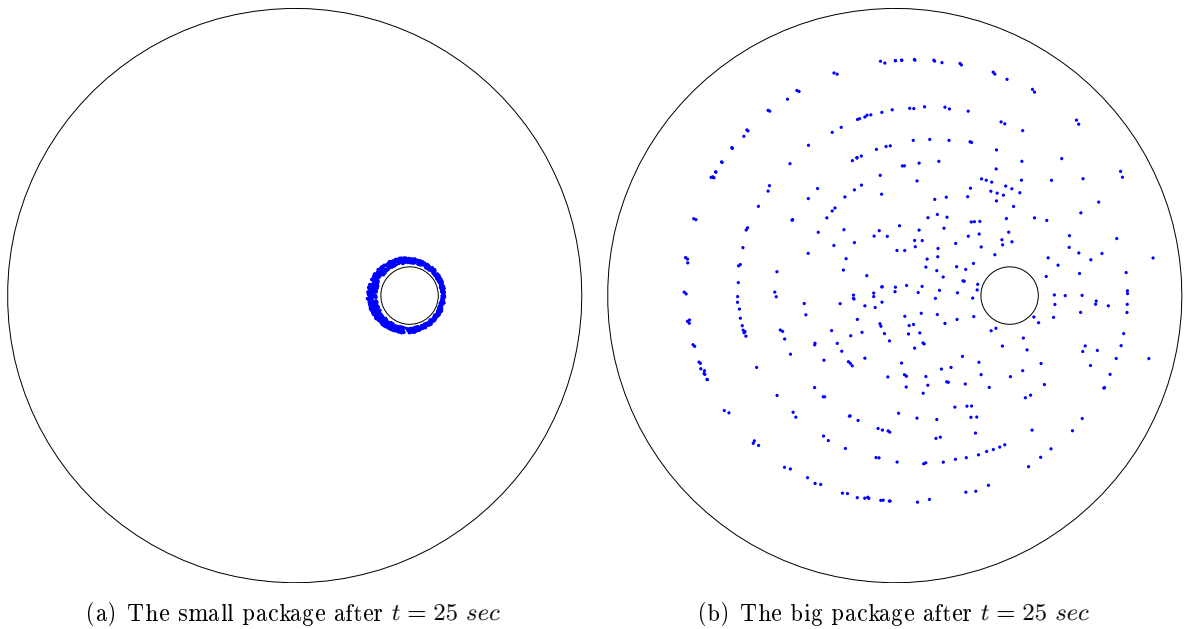


Figure 17: The statistical simulations for the 1600 rpm case at $t = 25 \text{ sec}$ (without the grid)

after a shorter ($t = 4$ and $t = 10 \text{ sec}$) time and and Figure 17 shows them at the end of the

simulations ($t = 25 \text{ sec}$) for the 1600 rpm case – the mixing process can be seen better by watching the attached videos. It can be seen on Figures 18, 19, and 20 that the blue coloured small package always has a wavier s^* , than the red coloured big package, while this waviness gets smoother and smoother in both cases. It is also remarkable that as the rpm increases, the transient part gets shorter. One can see the theoretical limits of the standard deviations for both packages on these figures (marked by dashed lines).

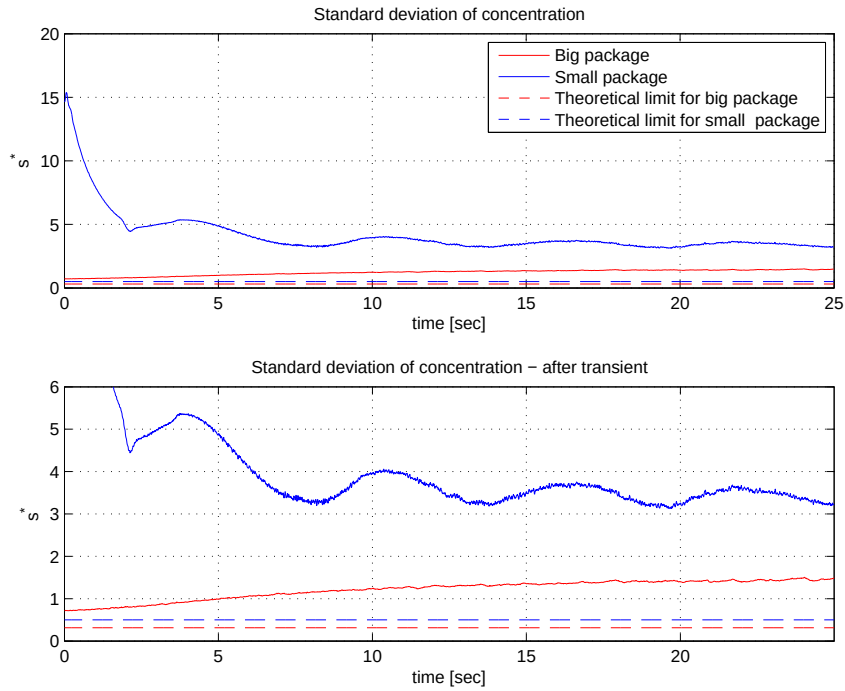


Figure 18: The achieved standard deviations for 100 rpm

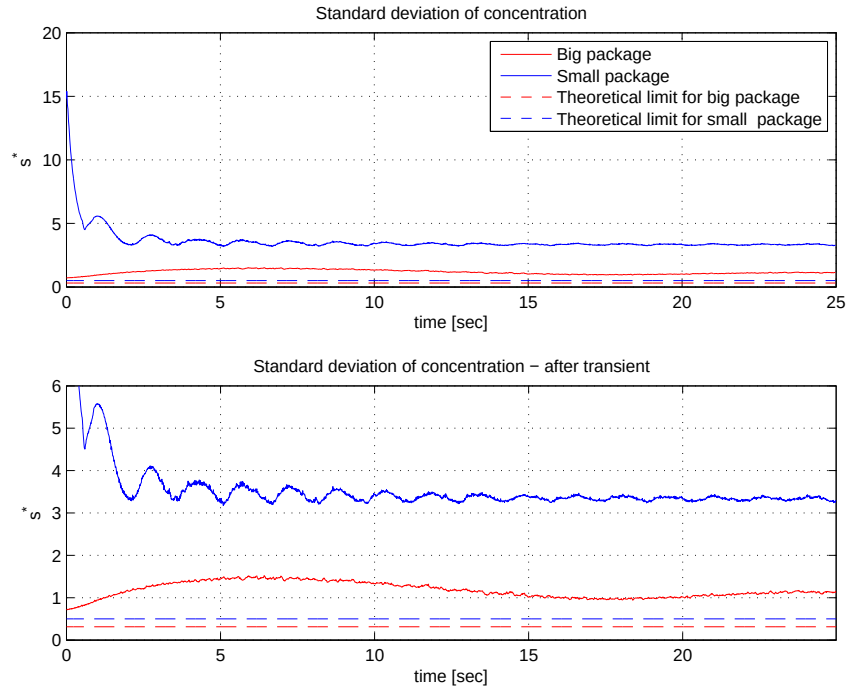


Figure 19: The achieved standard deviations for 400 rpm

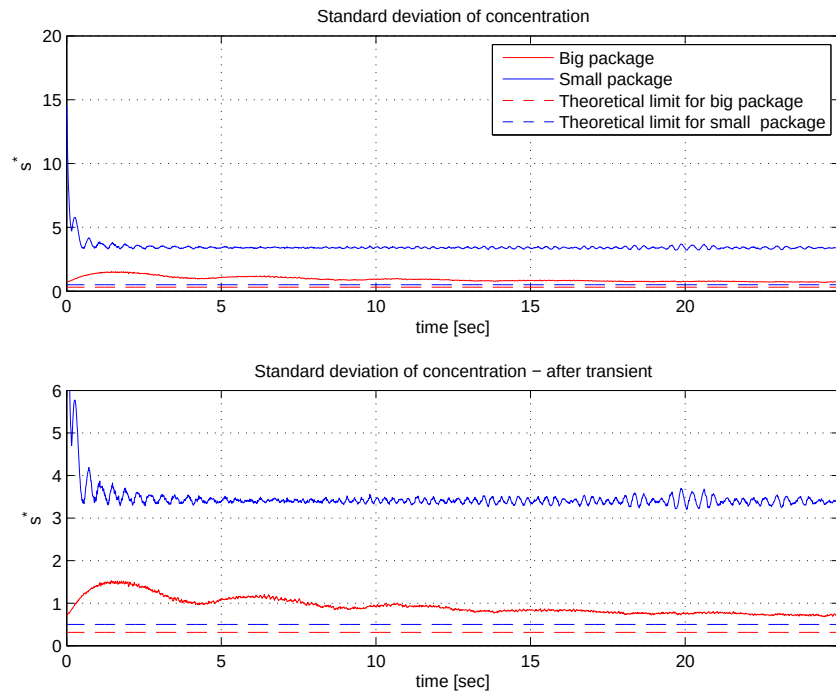


Figure 20: The achieved standard deviations for 1600 rpm

4.4 Principal deformations

We plotted a three dimensional contour plot of the calculated eigenvalues for every case – everywhere the bigger κ was used from the eigenvalue pairs.

Due to experiencing a large variation of the eigenvalues at the far-field zones, the natural logarithm of κ was plotted. It can be seen on the Figures 21, 22 and 23 that in the region $x \in [0.6; 1]$ the stretch is higher than on the other side of the stirrer – $x \in [-1; 0.2]$. It can be seen in this case as well that the highest revolution number gives the biggest eigenvalues. The density of the contours increases rapidly by approaching the vicinity of the stirrer, therefore that is the area where most of the stirring and stretching is done. It is clearly seen that there is a large variation (10 orders of magnitude) in the stretching properties of the flow field, leading to highly uneven “mixing”. Moreover, this kind of analysis does not give any piece of information on the reorientation and of the long-term mixing behaviour.

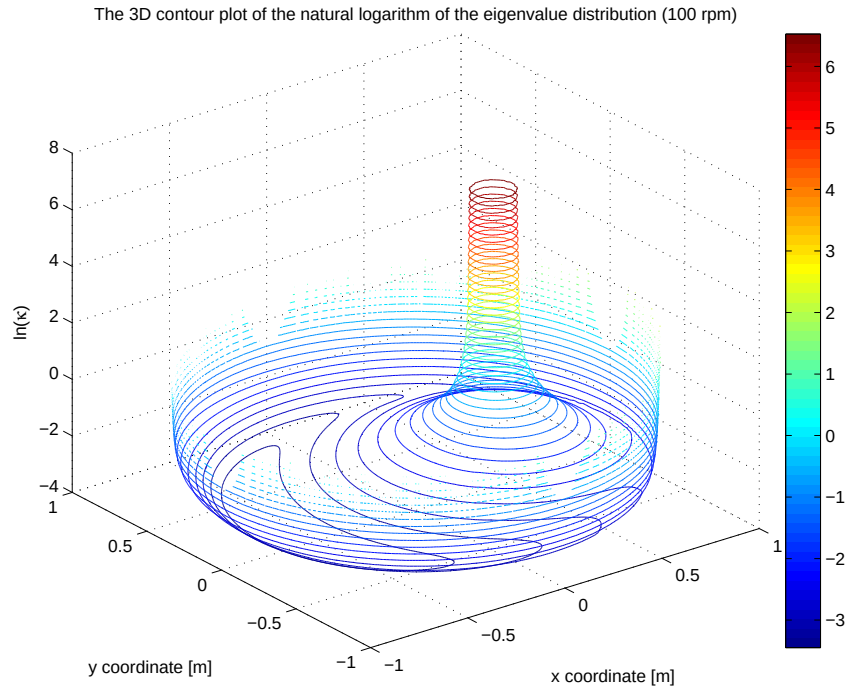


Figure 21: The 3D contour plot of the larger eigenvalues for the 100 rpm case

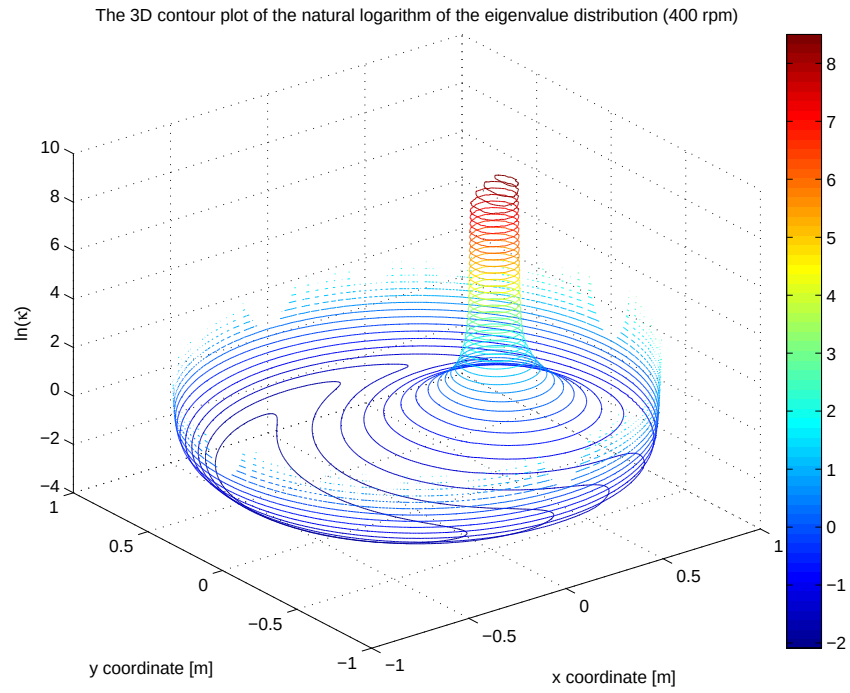


Figure 22: The 3D contour plot of the larger eigenvalues for the 400 rpm case

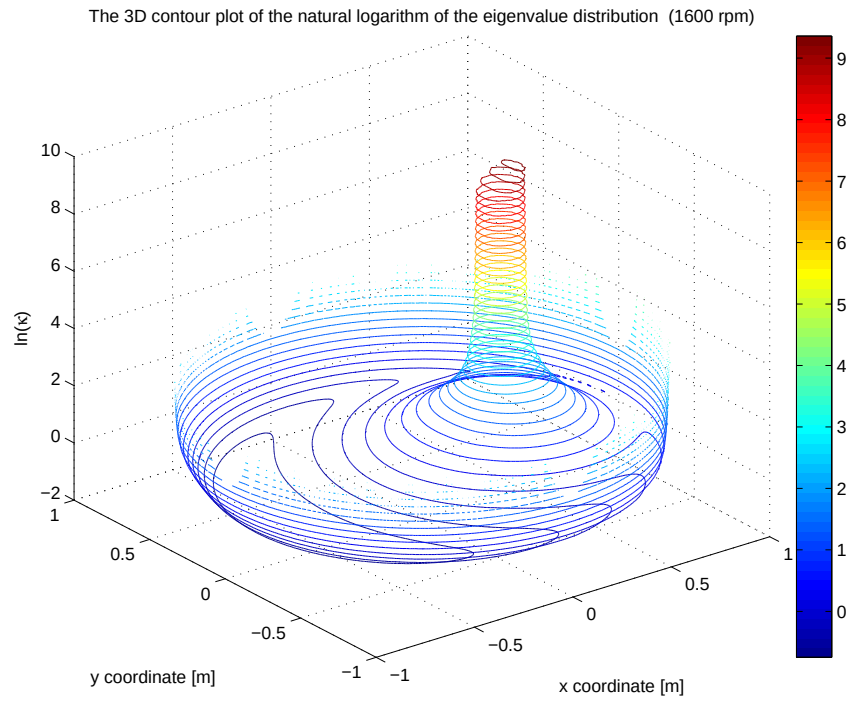


Figure 23: The 3D contour plot of the larger eigenvalues for the 1600 rpm case

5 Summary

This report summarizes the first steps towards developing measures to evaluate the mixing capabilities of 2D incompressible flow fields. At this initial stage, an extremely simple geometry was used consisting of a cylindrical tank and a rotating, circular stirring element located eccentrically. The velocity field (and the velocity gradients) were obtained with the help of carefully verified CFD computations.

It has to be noted that the actual flow field lacks of reorientation (which, besides stretching, is essential for good stirring); the streamlines are “almost” circular, thus we did not expect intensive mixing.

By tracing fluid packages, one not only visualizes the mapping of the flow but also is able to compute the global mixing efficiency $\eta = (d/dt) \ln(P(t)/P_0)$. We observed the same tendency that Ottino describes for “local” mixing efficiency; namely that for “good” mixing, one needs non-zero long-term value of the efficiency. The drawback of this technique is that to keep errors under an acceptable level, one has to increase the number of boundary points, which escalates the computation time.

The statistical approach seems to be a simple, natural and global way of measuring mixing rate, but again, the computational effort is enormous. One has to trace a large number of particles and the vast majority of the computational time is consumed by ordering the particles to cells.

Finally, having a look at the largest eigenvalues of the velocity gradient matrix (i.e. the strongest stretching) is simple, fast (the velocity gradients are provided by the CFD computation) but seems to be inadequate by its own as it does not carry any information on the reorientation. We speculate that it might be combined with streamline computation e.g. by continuously monitoring the angle of the tangent of the streamline and the eigenvectors of the velocity gradient matrix. One of our future plans is to perform such studies.

For future studies, it is important to introduce flow fields that are indeed capable of mixing. The simplest way seems to be to introduce several mixing elements and different stirring protocols, such as in [1]. Nevertheless, one should not forget that the main question remains how to connect a given velocity field to mixing “goodness”.

Budapest, January 4, 2013

.....
Máté Tibor Szőke

References

- [1] BOYLAND, P.L., AREF, H., STREMLER, M.: “Topological fluid mechanics of stirring”, *Journal of Fluid Mechanics*, vol. 403, pp. 277-304, 2000.
- [2] ANSYS INC., *ANSYS CFX Users Guide*, 2011.
- [3] ANSYS INC., *ICEM Users Guide*, 2009.
- [4] http://en.wikipedia.org/wiki/Finite_difference, October 24, 20112, 11:01 p.m.
- [5] http://en.wikipedia.org/wiki/Horseshoe_map, September 26, 2012, 8:33 p.m.
- [6] DR. LAJOS TAMÁS: *Az áramlástan alapjai*, Műegyetem Kiadó, ISBN 978 963 06 6382, 2004.
- [7] MATHWORKS INC., *Matlab Users Guide*, 2011.
- [8] J. M. OTTINO: “Mixing, chaotic advection, and turbulence”, *Annual Reviews of Fluid Mechanics*, University of Massachusetts, 1990.
- [9] J. M. OTTINO: *The kinematics of mixing*, Cambridge University Press, ISBN 0 521 36335 7, 1997.
- [10] http://en.wikipedia.org/wiki/Pigeonhole_principle, October 25, 20112, 18:42 p.m.
- [11] SZENTGYÖRGYI S.: *Vegyipari gépek II/1*, J-4489 Tankönyvkiadó Budapest, 1992.