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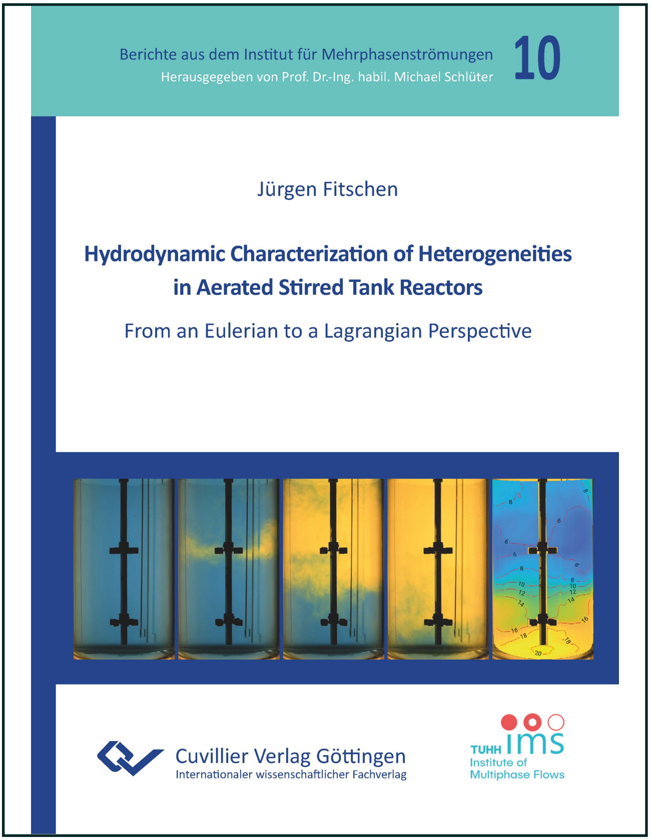
Hydrodynamic Characterization of Heterogeneities in Aerated Stirred Tank Reactors

From an Eulerian to a Lagrangian Perspective



Berichte aus dem Institut für Mehrphasenströmungen
Herausgegeben von Prof. Dr.-Ing. habil. Michael Schlüter
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Cuvillier Verlag Göttingen
Internationaler wissenschaftlicher Fachverlag

TUHH ims
Institute of Multiphase Flows

https://cuvillier.de/de/shop/publications/8716

1. Introduction

"*Bioreactor agitator engineering is a broad mosaic. The image is simple and clear from a distance, but as the viewer moves closer, a multitude of distinct individual pieces come into view.*" from Keith Flanegan.

The quote from Keith Flanegan impressively summarizes not only the historical background of stirred tank reactors, but also the current state of research in just one sentence. Stirred tank reactors have been used for centuries for mixing and homogenizing several substances. Whereas the focus was initially on the preparation of food and stirring was often uncontrolled, stirred tank reactors have become indispensable in modern process engineering [Kra14].

In modern processes in the chemical and biotechnology industries, various types of bubble columns and stirred tank reactors are widely used. In general, aerated stirred tank reactors are used for many applications and especially for shear-sensitive processes, such as the cultivation of mammalian cells. The use of stirred tank reactors is mainly based on the fact that, due to the mechanical power input by the stirrer, controlled operating conditions can be maintained with regard to important properties such as good heat and mass transfer as well as good mixing. Nevertheless, new processes are always developed on a laboratory scale to save time and resources. After a successful development phase, however, the process developed at laboratory scale must be scaled up to industrial scale. Especially when scaling up processes in stirred tank reactors, a good understanding of the operating behavior depending on the operating parameters such as the mechanical power input or the aeration rate can determine the success or failure of the scale-up.

For the successful scale-up of a stirred tank reactor, the initial system must be sufficiently known and characterized, and the right scale-up strategy must be selected. In particular, the choice of the scale-up strategy poses a great challenge due to the fact that not all system properties scale equally in the geometric scaling of stirred tank reactors. This is a great challenge, especially for multiphase processes. An impressive visualization of the dilemma that arises during geometric scale-up is shown in Figure 1.1 according to Zehner 2002 [Zeh02]. Using the example of the operating parameters of the dimensionless mixing time θ, the Froude number *Fr*, the stirrer tip speed u_{tip} and the stirrer Reynolds number *Re*, Figure 1.1 shows the dependence of the specific power input *P/V* for different orders of magnitude where one of the operating parameters is kept constant. It can be seen, that for a constant specific power input over various scales, other important system parameters cannot be kept constant. For example, for a constant dimensionless mixing time θ, the specific power input *P/V* must increase significantly. However, if the stirrer tip speed u_{tip} is to be kept constant, the power input *P/V* must be significantly reduced with increasing scale. This impressively illustrates the difficulties of the scale-up.

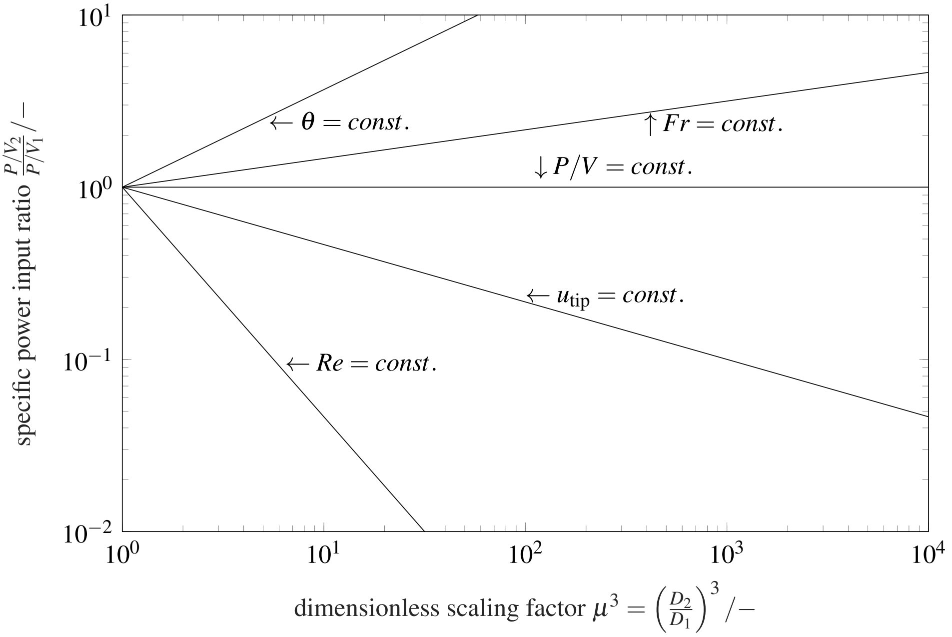

Figure 1.1. Dependence of the specific power input during scale-up of stirred tank reactors on the basis of various constant operating parameters for different tank diameters $D_1 < D_2$, according to [Zeh02]

Another dilemma is that although a large number of fundamental papers on the investigation and description of the operating behavior of stirred tank reactors have been published in recent decades and have thus made a significant contribution to the general state of the art today [Zlo01, Kra12, GO04, Mon15, Gez00, Mav01], even minor deviations from the investigated model geometries mean that the results in the literature can no longer be applied directly to other problems. This is shown particularly impressively by the example of the global mixing time of an aerated stirred tank reactor on an industrial scale by Rosseburg et al. 2018 [Ros18], because on the one hand, there is a lack of publications and thus of correlations to the mixing time behavior of stirred tank reactors on industrial scale, and on the other hand the geometric installations often do not correspond to the own scale-up. This leads to increased uncertainty during scale-up, especially for multiphase systems, whose operating parameters have complex interactions.

Furthermore, the classical characterization approaches for describing aerated stirred tank reactors usually use integral measured variables, such as the global mixing time or the global volumetric mass transfer coefficient. This method of characterization corresponds to the Eulerian approach. The Eulerian description refers to a stationary coordinate system for the description of physical processes. Here the observer is at a fixed location for the description of the environment. Whereas in the Lagrangian approach, physical properties are described using a moving observer, for example by a particle in a flow [Her06].

Since the motivation of this work is the further development of established measurement methods as well as the better understanding of heterogeneities in stirred tank reactors, the following topics are discussed. First, the required theoretical fundamentals about power input and mixing are given for the general description of the operating behavior of stirred tank reactors. Following this, the Lagrangian analysis methods are described, which are used to describe the mixing structures as well as the heterogeneities in the system. Furthermore, a transfer from the Eulerian to the Lagrangian description is shown, which provides deep insights into the prevailing transport processes in stirred tank reactors.

Due to the fact that local measurement methods for the flow field measurements and mixing time measurements used in this thesis require a high experimental effort, as well as a perfect and non-distorted optical access, the methods in this thesis are implemented and tested on a stirred tank reactor at laboratory scale. First, classical power input and mixing time characteristics are measured on the laboratory-scale stirred tank reactor and compared with the literature. This measuring procedure is used to validate the experimental setup and the used measurement methods. Subsequently, spatially resolved mixing time experiments are performed, and the results are discussed. Finally, Lagrangian particle tracking velocimetry is used to determine the local and three-dimensional flow field, and Lagrangian analysis of the local residence time and dispersion are shown. Following the laboratory scale results, an outlook on the extension to industrial scale stirred tank reactors is given.

2. State of the Art and Basic Knowledge

In the following, the fundamental theories as well as the state of the art on the design and characterization of aerated stirred tank reactors are described. First, the general design of aerated stirred tank reactors is discussed. Then, the fundamentals of power input and mixing time are discussed in more detail. Finally, Lagrangian approaches to describe the single-phase transport processes are described and discussed.

2.1. Reactor Design and Characterization

The following subsections first describe the fundamentals of stirred tank reactor design and the most important characterization parameters. On the one hand, typical geometric designs and their desired influence on the operating behavior of stirred tank reactors are discussed, and on the other hand, the problem-specific nomenclature is defined so that no misunderstandings occur. Subsequently, the theoretical fundamentals of specific power input, mixing time and Lagrangian analysis methods with respect to stirred tank reactors are explained.

2.1.1. Fundamentals of Stirred Tank Reactor Design

In principle, there are virtually no limits to the design of stirred tank reactors for mixing and homogenization tasks. Essentially, a stirred tank reactor consists of the basic elements of the stirred tank reactor, the stirrer shaft including stirring elements, a motor, baffles and a temperature unit. Moreover, the design of stirred tank reactors is standardized in DIN 28130 [Nor07]. However, the greatest design diversity depends on the dimensions of the individual components and their respective placement [Kre02]. Furthermore, a gas supply unit is required for multiphase gas/liquid systems. Based on the listed basic components, it becomes clear that a large number of different designs are possible due to the free combination and placement of the components in the system. Especially due to this variety of design possibilities, it is very difficult to find a comparable configuration in the literature that is suitable for new problems. For this reason, the most important theoretical fundamentals are explained and described in the following, using one of the configurations used in this work as an example for each case.

Figure 2.1 i) shows the basic components which are usually used for the design of stirred tank reactors. However, the number and the shape of the baffles and stirrers in the system can be freely selected. Baffles are used to intensify the turbulence and thus the power input in the system in the case of low viscosity media, as well as to avoid the formation of a trombe. In general, 3-4 baffles are used. In the case of 4 baffles, the system is also referred to as a fully baffled system [Zlo01]. The main dimension quantities are shown in Figure 2.1 ii). Basically, a fill height to reactor diameter ratio $H/D_{\mathrm{STR}} = 1$ is desined for standard processes.

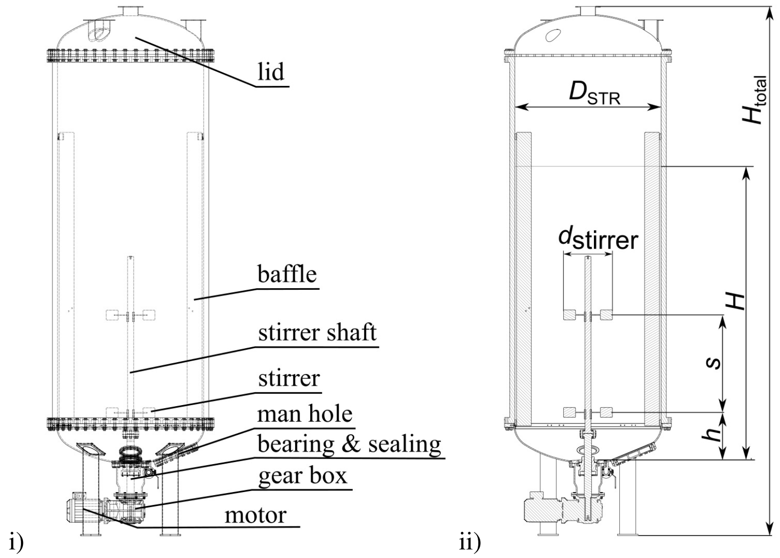

Figure 2.1. i) Sketch of the essential components of a stirred tank reactor; ii) main dimensions in relation to stirred tank reactors and their components

However, the tank diameter quickly becomes larger $D_{\mathrm{STR}} > 4.6\,\mathrm{m}$ with increasing reactor volume [Zlo01], which limits tank size due to transport constraints. Due to this, for industrial scale stirred tank reactors with a volume $V_{\mathrm{STR}} > 2\,\mathrm{m}^3$, a filling height to reactor diameter ratio $H/D_{\mathrm{STR}} > 1$ is used. However, this also results in disadvantages which have to be solved by changing the design. On the one hand, it is recommended to distribute several stirrers over the reactor height H for slim vessels. This means that the stirrer shaft must be longer and thus more stable. On the other hand, the mixing time increases accordingly with increasing filling heights to reactor diameter ratio $H/D_{\mathrm{STR}} > 1$ [Zlo01]. This must either be taken into account in the design or compensated for by alternative stirrer combinations.

For different purposes, a variety of stirrer types can be selected. In principle, the different types of stirrers can be divided into two categories. A distinction is made between axially and radially pumping stirrers. Figure 2.2 shows a typical radially pumping Rushton turbine (i)) and an axial pumping pitched blade stirrer (ii)).

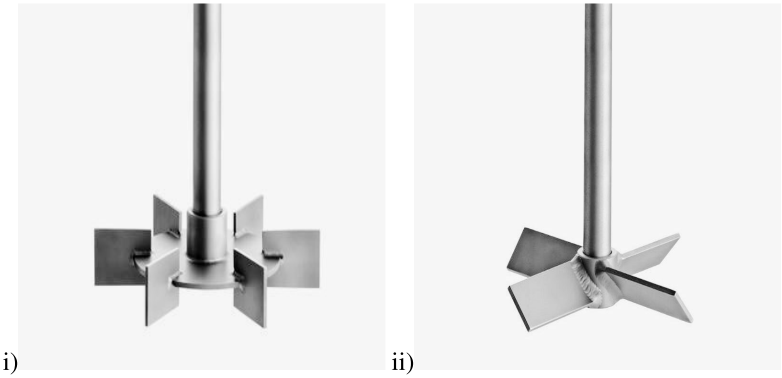
i)
ii)

Figure 2.2. Representation of the characteristic axially and radially pumping stirrer: i) Rushton turbine, ii) pitched blade turbine; photos from [Gmb21]

The predicted flow structures resulting from the use of the two stirrer types are shown in an idealized form in Figure 2.3. The structures shown refer in each case to an axially and a radially pumping stirrer type, as well as the combination of two of the respective stirrer types. The vortices shown as examples in Figure 2.3 start at the lower stirrer. The direction of rotation of the vortices is indicated by an arrowhead at the end of the vortices. Figure 2.3 i-ii) shows the predicted large-scale flow field of one or the combination of two axially pumping stirrers. The figure clearly shows that the liquid is drawn to the top of the stirrer and flows off axially. Subsequently, the liquid is redirected in the reactor bottom and deflected upwards in the area near the wall of the cylindrical reactor. Furthermore, it is obvious that the influence of the stirrer on the upper part in the system is not particularly large. In order to achieve a more uniform influence by the stirrers over the entire reactor volume, several stirrers are often placed on one stirrer shaft (see Figure 2.3 ii)).

The behavior of radially pumping stirrers like a Rushton turbine can be seen in Figure 2.3 iii). In radially pumping stirrers, analogous to centrifugal pumps, the liquid is sucked in the area of the axis of rotation and then transported radially outward. The volume moved

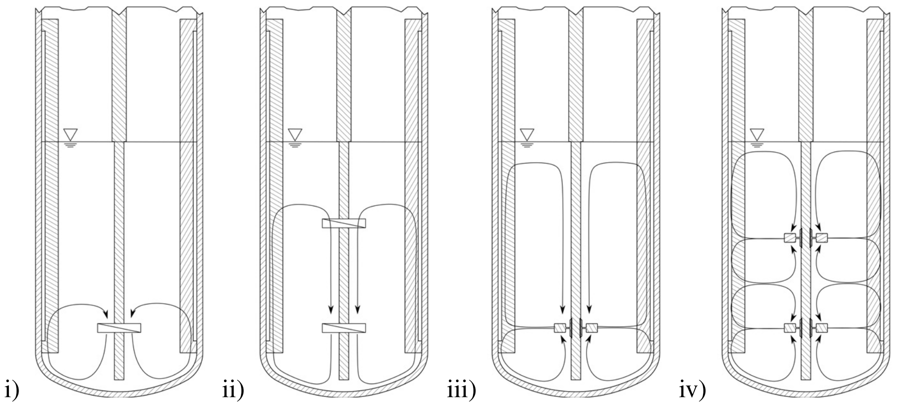

Figure 2.3. Representation of the characteristic flow behavior of a: i) single pitched blade turbine (down pumping), ii) double pitched blade turbine (down pumping), iii) single Rushton turbine and iv) double Rushton turbine

radially by the stirrer is then discharged downward or upward at the inner reactor wall. As a result, two characteristic vortices are typically formed in radially pumping stirrers. Due to this, the volume that is primarily influenced by the stirrer is larger than in comparable axially pumping stirrers. Nevertheless, even with radially pumping stirrers, several stirrers are often installed on the shaft to homogeneously distribute the power introduced into the system over the reactor height (see Figure 2.3 iv)).

In addition to the subdivision according to the main pumping direction, other important properties can be assigned to stirring elements. Table 2.1 provides an overview of which agitators are suitable for which process engineering tasks. Deciding which type of stirrer should be used is largely determined by the process engineering task. At this point, a distinction is made between suspending and dispersing two or more phases. The tasks are listed line by line in the first column. In the other columns, the respective basic stirrer types are listed and their suitability for the corresponding tasks is indicated. In addition to the process engineering task, the expected viscosity of the medium to be stirred is also important for the selection of the stirring elements because the range of influence of the stirrer decreases with increasing viscosity, so that the stirrers are consequently designed to be larger (see table 2.1 anchor and helical stirrer).

Furthermore, not all stirrer types are suitable for dispersing a gas/liquid or solid phase in an aqueous phase. For the dispersion of a second phase, high shear fields are required. Radially pumping stirrers are particularly suitable for this purpose. A special case is suspension,

Table 2.1. Selection guide for suitable basic stirrer types for various mixing and dispersing tasks, based on [Kre02]

typical stirrer	propeller	Rushton turbine	dissolver	pitched blade	anchor	helical
example						
pumping mode	axial	radial	radial	axial radial	radial	axial
homogenize	+	-	-	+	+	+
disperse gas/liquid	-	+	-	-	-	-
disperse liquid/liquid	-	+	+	-	-	-
disperse solid/liquid	-	-	+	-	-	-
heat transfer	-	-	-	+	+	+
viscosity range [Pa·s]	< 2			< 10		< 1,000
Preferred flow condition	turbulent			transition		laminar

which is a special form of solid/liquid dispersion, but the density of the solid is significantly greater than that of the liquid and thus the solid tends to sediment [Kre02].

As already mentioned, baffles prevent the formation of a trombe and increase the degree of turbulence in the system. They contribute to the intensification of the stirring task and thus to mass transfer in the system. Regarding heat transfer, for small amounts of heat to be removed or added, a simple double jacket reactor can be used, where the cool/hot medium circulates in the double jacket and controls the temperature in the stirred tank reactor via an external heat exchanger. For higher heat quantities to be removed or supplied, additional heating/cooling elements can be installed in the stirred tank reactor to intensify the heat exchange. Especially for temperature-sensitive processes, such as in the biotechnology industry, internal heat exchangers can improve the heat control by providing a significantly larger surface area compared to the double jacket [Zlo01]. However, the large surfaces of internal heat exchanger bundles also pose an increased risk of contamination, hence internal heat exchangers are not used in critical processes.

2.1.2. Fundamental Theory of Power Input

The following details on the power characteristics of stirred tank reactors refer only to single liquid phase operating. The theoretical fundamentals of the global power input in stirred tank reactors are discussed, followed by the fundamentals of local description of energy and turbulence by means of energy spectra.

Global Power Input

The following explanations are based on a dimensional analysis according to the Π-theorem [Zlo01]. With respect to the power input to be characterized, the power input P is set as the target value in the dimensional analysis. Figure 2.4 shows those parameters which have an influence on the power input. These parameters can be divided into geometrical (vessel diameter D_{STR} and stirrer diameter d_{stirrer}), physical (viscosity η and density ρ) and process-specific properties (stirrer frequency n). The Π-theorem states that the correlation of α physical quantities characterizing a system can be reduced by γ dimensionless numbers . The number

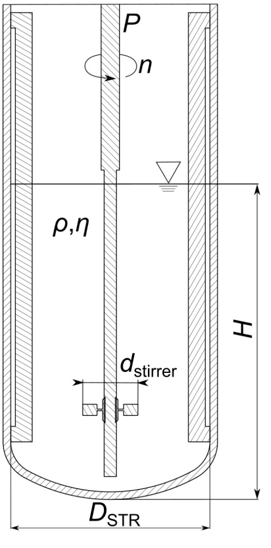

Figure 2.4. Main dimensions of stirred tank reactors and main unaerated properties; tank diameter D_{STR}, stirrer diameter d_{stirrer}, viscosity η, density ρ, stirrer frequency n and power input P

$$\gamma = \alpha - \beta \tag{2.1}$$