Chapter 1

Introduction and Scope

1.1 Introduction

Baker's yeast has a variety of fields of application. It is primarily used in bakeries as baking agent and as taste donator. Another growing field of application is the food industry in general using yeast extracts. In agriculture, the high protein content makes yeast an important part of modern animal feed. The nitrogen content is a reason for also using yeast as fertilizer. Beside these common areas, current research attempts to extend the applicability of yeast. An interesting example is the use of dead yeast cells to create hollow pigments for paper industry [147].

Yeast as a low price product requires efficient production in huge amounts. Therefore, in production large reactors with operation volumes up to several hundred cubic meters are used. Molasses as by-product of sugar industry usually serves as substrate. Without exception, production reactors are air-lift type reactors. They combine both, ease in handling because of only a few internal installations and a good mixing and aeration performance at relatively low energy input. Reactors are generally designed as bubble columns or air-lift loop reactors with static or dynamic gassing systems.

Installation as well as running costs are major reasons for decisions for a certain reactor type. Energy cost for oxygen support hold the principal share of running costs. On the one hand, the cost for buying a reactor are generally higher for dynamic in comparison to static gassing systems. On

the other hand, dynamic systems may show supreme energy efficiency and can thus help to reduce running costs [53]. With increasing environmental standards, the comprehensive efficiency of running and planned systems will win its share.

International pricing pressure with respect to the product yeast especially challenges industrialized nations where energy prices are at elevated levels and environmental standards increase running costs.

Industrial yeast strains have extensively been improved. Basically only changes due to different substrates are still subject of investigation. The yeast market is saturated or even oversaturated. As a consequence, optimization via market volume is not possible. Currently, yeast is delivered as block, as granulate, dry and as liquid to serve the special needs of customers. Increasing yeast quality and shelf life is taken for granted and cannot serve as argument for a rise in price. Thus, the only realistic way to increase international competitiveness is to reduce the running costs. First, the comprehensive need for energy has to be minimized and second, oxygen and mixing yield have to be maximized.

Understanding the flow characteristics, the reactive processes and the combination of both is substantial for optimization of yeast reactors. The aim is to produce with highest yield at lowest energy consumption. Therefore, mass transfer has to be enhanced. At the same time mass transfer is a complex function of the bubble size distribution, the mass transfer coefficient and thus, a function of the physical properties of the fluids. For a given set of fluid properties, also the gassing system and the operation conditions have their indirect share on mass transfer.

1.2 Scope of the Work

Coupling of multiphase fluid dynamics and biological growth is a common area of application in process engineering. The use of computational fluid dynamics in combination with growth models allows for general applicability to different reactor systems. Physics, biology, geometry and conditions are separately described.

Yeast cultivations last up to 24 hours. During cultivation parameters such as gas flow rate and volume may change. Accordingly, flow characteristics also change. Fluid dynamics and growth cannot be taken as being constant.

The direct interaction of fluid dynamics and growth requires combined simulations.

Related time scales differ and generally challenge to combine computational fluid dynamics and biological growth. While major changes in fluid dynamics happen within milli seconds to seconds, changes in growth may take hours to days. A direct co-simulation of this problem is not feasible.

The aim of this work is to develop a method to sequentially combine fluid dynamics and biological growth. Exemplary application in this work is baker's yeast production. Fluid dynamics are simulated with the commercial code CFX 11.0 by Ansys. The biological part has been implemented in Matlab and Simulink R2008a by Mathworks.

A 200 L reactor system is the basis for validation of simulated fluid dynamics and growth. The reactor is a bubble column with jet tubes as gassing system. This system has been chosen in relation to commonly applied industrial gassing systems. Axial liquid velocity serves to validate the fluid dynamics module. A cultivation experiment serves for validation of the growth model and the framework of sequential co-simulation. In contrast to industrial yeast production glucose directly serves as substrate.

Simulation of multiphase flow for reaction volumes above about five cubic meters is not practicable at the present time since element numbers rise up to billions. It is up to research and development in future decades.

Chapter 2

Fluid Dynamics and Simulation

2.1 Bubble Column Reactors

Bubble column reactors are vertically oriented cylinders with generally circular cross section area. Bubble columns are filled with liquid or liquid and solid to a certain level and aerated in the bottom section of the column.

These systems make use of the density difference between aeration gas and the liquid inside the reactor. The density difference in the gravitational field makes the gas bubbles rise. The slip velocity between gas and liquid causes drag forces and liquid motion is induced.

In general, bubble column reactors have only a few internal parts. As a result, their design is simple and cheap [93]. Being very easy and fast to clean is one of their greatest advantages.

In addition to fluid motion induced by bubble drag, fluid motion may be enforced. This directly influences the mean residence time of gas bubbles and may also increase oxygen utilization. As important as residence time are especially the total height of the column, the coalescence behavior in the adjacent multiphase mixture and the bubble size [120].

Additional parts may be installed in the bubble column in order to direct liquid and gas flow. The most common example is the group of airlift loop

reactors. The basic concept of such internal or external installations is the separation of liquid up- and down-flow regions.

In comparison to simple bubble column reactors, loop reactors may be operated with less energy input. Net draft tubes are used to even enhance mixing performance [57].

There are bubble columns of almost any size with volumes from some cubic centimeters up to about twenty thousand cubic meters. After decades of intense research on bubble columns the complete physical behavior is not entirely understood. Even though researchers have been trying to come up with general rules for scale-up [89, 135, 34, 137], up to now no general scale-up method is known which holds true for a relevant range of size.

Industrial application of bubble column reactors is as wide as their range in size. Typical areas are food production, chemical and biotechnological industry, processing and refinement of raw materials and waste water treatment [138, 46].

There are two basic concepts of gassing systems, static and dynamic. Static systems such as sparger plates, sieve plates and sintered plates are known to produce larger bubbles due to their position at the bottom of the reactor [133]. The change of flow direction at the bottom causes major radial velocity components and thus increased bubble coalescence in this area. A number of single vertically oriented nozzles as well as horizontally oriented tubes with holes or membranes and a distinct distance to the bottom of the column [29, 131] show much better performance.

Dynamic systems defined in the classical way are mainly injector and ejector nozzles [23] or liquid jets applied to the free liquid surface similar to sprinkling systems [23, 120]. The latter type of system is still used for oxygenation of biological systems with relatively low oxygen consumption. The modern definition of dynamic gassing systems relates to systems with moving parts such as rotors with openings on their surface [13, 96, 53]. The dynamic pressure at certain areas of rotating parts reduces the local pressure such that gas is intaken with low or even without positive primary pressure.

In combination with additional installations for bubble distribution, such systems reach very homogeneous gas distributions, small bubbles and good mixing performance. Additional parts impede cleaning. Up to now, no generally accepted optimum gassing system is known.

The bubble size distribution depends upon used liquids, solids and gases, the gassing system, the gas flow rate, the column dimensions and even more factors. At the same time, this distribution causes a certain gas holdup and

the related liquid flow field [93]. The effects are coupled in a complex manner which makes research especially on scale-up as difficult as it is.

2.2 Multiphase Flow in Simulation

In bubble column reactors a continuous liquid phase is gassed with a dispersed gaseous phase. The holdup or volume fraction characterizes whether a phase is regarded to being continuous or dispersed [75].

The complexity of model description increases with increasing number of phases. In practice, the number of adjacent phases is reduced to the smallest physically meaningful set. In bubble column reactors for yeast production there are a liquid and a gas phase as well as a solid phase representing yeast cells. Since yeast cells have a diameter of 5 to 10 μm and a mass density very similar to water, in approximation the solid phase can be omitted for most simulations. Yeast cells almost perfectly follow the flow and do not significantly change flow characteristics. The suspension is treated as one pseudo phase with fluid characteristics of water.

Oxygen is one of the central components for yeast growth of interest in this case, thus oxygen has explicitly to be taken into account in the simulation. Oxidative yeast growth consumes oxygen while producing carbon dioxide. Oxygen is transferred from gas into liquid phase and carbon dioxide leaves the liquid in the opposite direction. For simplicity reasons, the number of oxygen molecules entering the liquid phase is assumed to be of the same order as the number of carbon dioxide molecules leaving it. Accordingly, volume changes in the gas phase due to biological growth are negligible.

Bubble column reactors obviously show three dimensional and time dependent flow fields. Nevertheless, time averaged information corresponds to a probability of occurrence and thus gives hints for optimization. It is common sense that the transient character of the flow field also has to be taken into account. The flow field is characterized by its unsteadiness and the turbulence.

Computer resources limit computational fluid dynamics. In order to simulate systems of relevant size, first approaches have therefore been reduced to two dimensions. Such a simplification is allowed when the system has at least one almost infinite dimension not being the main flow direction. This dimension may often be omitted without the loss of important information.

Even though columns with rectangular cross section do not fulfill this requirement, literature shows that researchers often neglect the direction of lowest extension [20, 11]. The assumption of two dimensionality is not justified in most simulations of bubble columns but especially not for those with a circular cross section area [49, 105, 91, 30, 126, 54, 115]. Continuity requirements must provide different flow fields for columns with rectangular and with circular cross section area. Most systems of industrial relevance do have a circular cross section area.

The top region of bubble column reactors is filled with the gas leaving the mixture of gas and liquid. This interface in the top region between gas and the mixture of gas and liquid is called free surface. It is not a sharp boundary. Simulations with free surfaces in heterogeneous multiphase systems give rise to severe difficulties. As long as the free surface is not of special interest it can be approximated by a plane surface where no shear forces occur. Thus, the computational domain can be reduced to the region captured by the gas liquid mixture. This method is generally accepted [86, 11, 115].

2.2.1 Simulation Approaches

There are two main approaches in simulation of multiphase flow. The first approach deals with descriptions of systems where one finite volume element may contain more than one phase. This kind of description is named disperse and is known as Euler-Lagrange or Euler-Euler [44]. In the second approach the phase boundary is tracked for all cells [78]. Descriptions of this kind are therefore named separated. The best known description is the Volume of Fluid method.

The Euler-Lagrange method treats the dispersed phase as separated particles of zero volume. The trajectories for every single particle are calculated based on the main flow field of the continuous phase [44]. This method gives insight into dispersed phase flows [43]. The approach suffers from computational demand. Therefore, simulations using the Euler-Lagrange approach are limited to a number of some thousand dispersed phase particles. Bubble columns with millions of bubbles per cubic meter cannot realistically be described.

The Euler-Euler method is also called two fluid or multi fluid method. The different phases are treated as inter-penetrating continua [44]. Thus, this method does not account for direct particle interaction. There is a mass and momentum conservation equation for every fluid. The volume fraction

of every single phase is calculated for all volume elements [125]. The Euler-Euler method is applicable for high volume fractions of the dispersed phase. Its computational demand is relatively modest. This is the main reason for the wide usage of this approach [126].

In contrast, the Volume of Fluid method captures the shape and even the shape deformation of single dispersed particles [43, 79]. Obviously, it is the physically most realistic way of simulating multiphase systems. The method has been applied to single bubble motion as well as to bubble interactions [15]. It is a great tool to study principle behavior of bubbles and to deduce advanced drag, break-up and coalescence models [15]. At the same time, it is computationally so demanding that only a few bubbles can be simulated at the present time. As a consequence, the Volume of Fluid approach suffers from similar limitations as experiments. Up to now, this method has not come up with overall better performing models.

2.2.2 Bubble Size Classes

The discussion about one definite bubble size versus bubble size distributions is as old as simulation of bubble columns. In real systems independent from the flow regime, there is always a bubble size distribution. Gas holdup, surface tension as well as influencing surface active agents and forces entail distributions of different sharpness. In simulations bubble size classes represent bubble size distributions. In most cases, bubble size is kept constant for every single class over the entire reactor.

Simple approaches use one averaged bubble size where averaging is problem related [126]. It has been shown that one single bubble size does not always capture flow physics [16]. Thus, researchers often apply two bubble size classes [81, 138, 101, 115]. These classes may interact with each other but also may coexist without interaction still enhancing the results. The assumption of two bubble size classes representing the distribution adequately results from dynamic disengagement experiments for aqueous systems [119, 68].

Population balances based on breakup and coalescence models are used to most realistically represent bubble size distributions [32]. Restricted computational resources often demand for simplified models based on the idea of population balances. An early approach is a kinetic model for the bubble rise velocity based on experimental knowledge [68]. The bubble size distribution might for example also be reduced to a local mean bubble size [32]. Other researchers use population balances to calculate bubble size distributions and

to reduce those to a finite number of bubble size classes. In a second step, the classes are used for Euler-Euler simulations [101, 115]. This approach is similar to the use of experimentally determined representative bubble size classes [54, 149].

Up to now, most implementations of population balances capture effects such as mass transfer but do not account for interphase forces based on local bubble size distributions. Instead, one single rise velocity is assumed for all bubbles. For correct simulations of the flow field, the interphase forces such as the drag force are of special importance. The first serious approach of taking into account such detailed interaction has been published in 2008 [18].

2.2.3 Bubble Drag

The drag force is the most important one acting between the continuous and the dispersed phase [32]. The fact that both phases are fluids results in possible motions inside the bubble and in generally deformable surfaces. Gas compressibility, viscosity and surface active forces make the system very complex.

There is no general applicable or accepted model for the drag force accounting for all known effects in any system. Most models are based on experiments or detailed simulation of very few bubbles [15]. They are therefore restricted in their application. Complexity on the one hand and the major importance of the drag force for simulation on the other hand are the present challenge in simulating bubble column reactors [16, 32].

2.2.4 Bubble Induced Turbulence

Bubble induced turbulence is the influence of moving bubbles on continuous phase turbulence [24]. Bubbles may increase as well as decrease the level of turbulence by their flexible surface and their wake structure depending on the flow [126]. Even though models for bubble induced turbulence have been developed for decades, the deduced models are still suffering from not understanding the exact physics behind.

There are three basic approaches to describe bubble induced turbulence in bubble column reactors. The first approach accounts for bubble induced effects by superposition of a shear and a bubble induced term for the effective viscosity [114, 112, 113, 92]. The additional term is taken to be proportional to gas holdup and slip velocity. The second approach assumes bubbles to