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3D CFD simulation of bottle emptying processes

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ABSTRACT

A 3D Computational Fluid Dynamics (CFD) approach is used to investigate the effect of parameters such as bottle geometry, surface tension, or inclination on bottle emptying processes. The method can e.g. be used to assess changes of bottle emptying times induced by new bottle shapes, and it is shown to be much more accurate than existing empirical models. While expensive commercial CFD software has substantially restricted and hindered the use of this method in the past, our approach is based on freely available open source CFD software and hence accessible to everyone.

1. Introduction

The simultaneous flow of several liquids through a single outlet of a vessel is important in many industrial applications. This study focuses on the bottle emptying process. In processes related to the rinsing, filling or cleaning of bottles, it is often important to control the flow regime within the bottle, and in particular to minimize bottle emptying times. Significant reductions of bottle emptying times help to reduce plant sizes and overall costs.

In 2007, a total volume of 33 billion liters of water was consumed in the US, and this volume was mainly filled into PET-bottles (Gleick and Cooley, 2009). The worldwide trend towards PET-bottles is also reflected by the fact that many new bottle geometries have been created in the last years, which can be easily realized in the commonly used two-step PET-bottle production process. In this process, the blow molding machine brings the PET-performs into almost every desired form (Lee, 2007). Undoubtedly, on the other hand, the geometry of a bottle affects all industrial processes related to the flow regime within the bottle, and hence producers need detailed information on the effects that bottle geometry variations may have on their processes.

Computational Fluid Dynamics (CFD) is particularly well suited to provide this kind of information since this technology can be used to investigate a large number of geometries in "virtual experiments" on the computer. Today, a CFD analysis allows the reproduction of local details in complex three-dimensional domains as well as the treatment of processes involving complex multiphysical phenomena such as multiphase, turbulent and reactional flows (Silva et al., 2008). Norton and Sun (2006) underline the benefits of using CFD in the food industry and provide a state-of-the-art review of various CFD applications that have already been used in the food industry. While bottle emptying processes have not yet been studied in terms of CFD simulations, a recent CFD-based investigation has analyzed the effects of bottle outlet diameters on drinking ease (Chihara et al., 2009).

Using other methods than CFD simulations, the flow pattern through a bottleneck or a single outlet has already been investigated by several authors in the past 50 years (Kolodziejski et al., 1996; Tehrani et al., 1992; Whalley, 1987, 1991; Wallis, 1961; Kohira et al., 2007). In 1961, Wallis introduced the dimensionless flooding parameter *C* for the flooding and emptying behavior of a bottle. Whalley (1991) and Tehrani et al. (1992) obtained a more realistic approach based on a correlation of the counter-current flow process with the Wallis-parameter *C*. In Tehrani et al. (1994), it was found that an increase of water temperature significantly decreases the emptying time (Table 1).

As discussed in Tehrani et al. (1994), temperature has two different effects mainly on the water phase: a decrease of viscosity (which tends to reduce the emptying time) and a decrease of surface tension (which tends to increase the emptying time). As the experimental data in Table 1 suggest, the viscosity effect seems to dominate the surface tension effect, which results in decreasing emptying times with increasing temperatures. Nevertheless, surface tension effects

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Table 1
Emptying times for various bottle parameters and temperatures obtained by Tehrani et al. (1994). Hundred percentage refers to the 15° C emptying times.

Bottle parameters			Emptying time			
Nr.	Volume [mL]	Neck diameter [mm]	15 °C [s]	30 °C [%]	60 °C [%]	93 °C [%]
1	1550	19.6	27.4	96.0	93.0	84.0
2	1520	20.6	19.9	95.0	93.0	87.0
3	2900	15.0	64.21	97.5	92.4	84.0
4	2900	28.0	14.5	98.5	93.0	82.0

instead of viscosity effects are investigated in this study since surface tension can be easily modified by the addition of surfactants e.g. in cleaning processes, while it is often more difficult to change the viscosity e.g. by temperature modifications which typically affect many other parameters of a process. Hewitt (1982) investigated the effects of bottle inclination. He compared bottles inclined between 30° and 45° with bottles inclined at an angle of 90° and found shorter emptying times in the 30–45° experiments (Whalley, 1991). Most other studies in this field relate to the rising velocity of the gas phase, the size of the outlet, the behavior of the aforementioned coefficient C depending on the geometry of the neck, or to the properties of the fluid and of the gas phase (Clanet and Searby, 2004). All these studies were based on bottle shapes as they were used at the time when the studies were performed, or on idealized bottle shapes essentially consisting of a piece of pipe closed at the top and with a hole at the bottom side. Nevertheless, these studies provide a first order of magnitude for the total filling and emptying times, which applies even for today's bottle shapes as will be shown below. A newer investigation performed by Skakauskas et al. (2006) basically confirms the results of the earlier papers.

Schmidt and Kubie (1995) performed experiments showing that the average liquid discharge velocity is independent of the liquid level in the vessel as well as of the shape of the outlet. They found a slight increase of discharge velocity with increasing vessel diameter and outlet diameter. The outlet diameter has a large impact not only on the outflow volume for a given discharge velocity, but also on the general flow pattern. The flow map in Fig. 1 shows qualitative water flow patterns depending on the outlet diameter (Kohira et al., 2007). As can be seen, there is no flow for $d < 4$ mm due to surface tension effects. In the region of counter flow ($d > 20$ mm), the outlet provides enough space so that water and air can pass each other simultaneously in the in- and out-flow directions. The oscillatory flow pattern refers to outlet diameters between 6 and 16 mm, and is characterized by four (cyclic) stages as follows: liquid downflow, bubble rise, repressurization, and refill. These stages will be discussed in more detail further below. Since most drinking bottle outlets have diameters between 16 and 24 mm, the oscillatory and counter flow patterns are most important in practice. The oscillatory flow pattern has already been investigated by Tehrani et al. (1992) referring to tank draining.

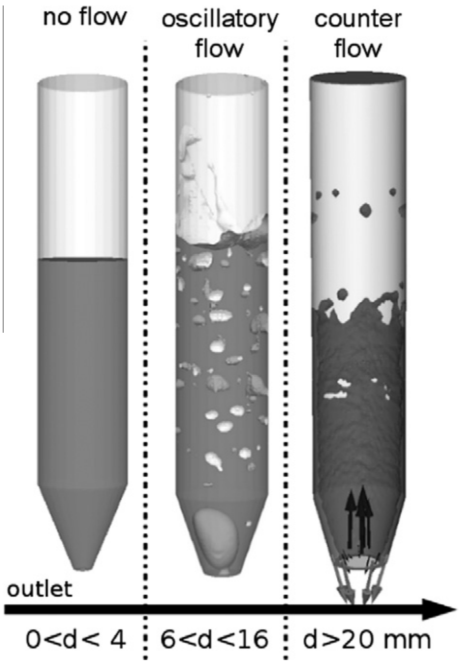

Fig. 1. Qualitative flow pattern depending on the outlet diameter, d [mm] (Kohira et al., 2007).

Our study is intended (a) to develop a CFD model of bottle emptying processes, (b) to achieve a better understanding of these processes based on the model, and (c) to apply these findings to answer some questions of practical relevance relating to bottle geometry, inclination and surface tension. Data from our own experiments are used for validation. The development of a CFD model for bottle emptying is a complex task due to the fact that this process involves highly turbulent, transient and three-dimensional two-phase flows. Based on an approximate pipe-shape model of the bottleneck, it can be shown that the dimensionless Reynolds numbers exceeds a level of 15,000. Beyond this, the transient turbulence pattern within the bottle is affected and intensified by the rising bubbles, and hence even more turbulence can be expected than is usual at this Reynolds number level.

2. Materials and methods

2.1. CFD model

For turbulent flows, the best simulation approach in the sense of accuracy is direct numerical simulation (DNS). In the DNS approach, even the smallest turbulent eddies and the fastest fluctuations are computed in detail, and hence extremely fine meshes and very small time steps are necessary to get a solution (Versteeg and Malalaseekera, 2007). As a consequence, DNS computations usually need a substantial amount of resources in terms of time and hardware requirements. An example is discussed in Versteeg and Malalaseekera (2007) where approximately 2.5×10^9 cells are required to simulate a process involving a Reynold's number of 15.000 ($N \cong Re^{9/4}$). For problems of this size, several months of computation time may be necessary even on parallelized supercomputer systems. The most popular way to avoid such unacceptably long computation time is based on statistical averaging approaches for the turbulence phenomena such as the Reynold's averaged Navier Stokes equation (RANS) (Versteeg and Malalaseekera, 2007). This technique is based on the assumption that the spatial distribution of the flow pattern in turbulent regions can be described by simplified models, which means that coarser meshes and bigger time steps can be used to compute the turbulence phenomena. In this study, hex-dominant meshes as described in Frey and George (2008) with 106,000–156,000 cells were used. Since computation times in CFD models depend exponentially on the number of grid points, this leads to a substantial