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Transient boundary condition approach for simulating mechanical mixing in large wine tanks

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ABSTRACT

Since wine is not continuously stirred during or after fermentation, it is common to use movable mixers on a variety of tank sizes or to install small, fast-rotating propeller mixers in large tanks. Many practically relevant optimization problems relate to processes occurring directly after the start of the propeller (flow field initialization period), which require 3D instationary models if CFD simulations are used. Based on traditional instationary models, these simulations are very time-consuming even on fast computers and limit the part of the flow field initialization period that can be computed. In this work, a new method was developed to speed up the transient simulation of mechanical mixing in large wine tanks. The method uses the traditional CFD techniques of moving reference frame (MRF) and several ensuing propeller rotations using sliding mesh (SM), to calculate a steady-state flow field and to compute the flow behavior in the propeller region. Subsequently, the flow's key figures are extracted for the propeller region at multiple time-points during one rotation and continuously mapped to a new simulation starting from a flow field with zero velocity. This new approach using a transient boundary condition (BC), was validated with tank mixing experiments and literature data. In contrast to the MRF method, it allows e.g. for an estimation of minimum mixing times similar to the SM method, while computation times are reduced by a factor of up to 20 for tank-mixer scenarios evaluated in this work. For a mixing simulation in a wine tank, the new method takes only 3 days compared to more than 60 days using the traditional SM approach.

1. Introduction

1.1. Mixing in the wine industry

Mixing is important throughout the wine production process (Boulton et al., 2013). During fermentation, CO_2-driven bubble mixing is used in most situations except for large tanks beyond 60,000 L (Schmidt and Velten, 2016). Before and after fermentation, mechanical mixing is used e.g. for sugar additions, nutrient additions, blending, fining, sulfuring or when reducing CO_2 (Cullen, 2009). Additives that need to be distributed homogeneously throughout the liquid are typically poured in from the top of the tank or pumped into the must or wine through side valves. Their volume and viscosities may vary greatly depending on the process.

Mobile tank-mixers are used in many cases and can be installed on the side of the tank through a one-way valve. Typically, these mixers are used for a variety of tank sizes and shapes, although it is not well understood how mixing parameters should be adjusted to achieve sufficient mixing of the whole tank for any particular tank-mixer configuration. Even large companies rely on estimations and empirical values which are neither validated nor optimized. This causes avoidable costs associated with a waste of energy, if mixing is too long, or with the clogging of filters and an inhomogeneous end product, if mixing times are too short. Beyond this, product quality may suffer both from too long mixing times (e.g., caused by the release of CO_2 or wine oxidation) and too short mixing times if, e.g., the concentration of important additives is too high or too low depending on the position in the tank.

1.2. Mixing simulations in CFD

For CFD simulations of mixing flows in turbulent regimes, several techniques have been developed based on the finite volume method (FVM). Blackburn et al. (2000) suggested to use blade element theory in combination with CFD simulations to estimate the velocity profile imposed by a propeller mixer. For this approach, however, the dimensionless lift (C_L) and drag (C_D) coefficients of the blade section, as well as, axial velocity profiles in the blade region must be known or measured prior to the CFD simulation.

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Nomenclature

C_1,C_2,$C_{3,RDT}$	coefficients (dimensionless)
C_D	drag coefficient (dimensionless)
C_L	lift coefficient (dimensionless)
C_μ	constant for eddy viscosity (dimensionless)
D_hub	hub diameter (m)
$D_\mathrm{propeller}$	propeller diameter (m)
D_vessel	vessel diameter (m)
$H_\mathrm{propeller}$	propeller clearance (m)
H_vessel	vessel height (m)
W_baffle	baffle width (m)
W_blade	propeller blade width (m)
σ_ϵ	turbulent Prandtl number for ϵ (dimensionless)
σ_k	turbulent Prandtl number for k (dimensionless)

Parameters

μ	dynamic viscosity ($\mathrm{N\,s\,m^{-2}}$)
μ_t	turbulent eddy viscosity ($\mathrm{N\,s\,m^{-2}}$)
ρ	fluid density ($\mathrm{kg\,m^{-3}}$)
τ_{ij}	shear stress (Pa)
G_k	generation of k due to mean velocity gradient
p	pressure (Pa)
ω_int	sampling angle interval (°)
t_int	sampling time interval (s)

Variables

u_i	velocity component (where $i = 1{,}2{,}3\ \mathrm{m\,s^{-1}}$)
u_j	velocity component (where $j = 1{,}2{,}3\ \mathrm{m\,s^{-1}}$)
x_i	coordinate direction (where $i = 1{,}2{,}3$ m)
x_j	coordinate direction (where $j = 1{,}2{,}3$ m)
f	rotational frequency (Hz)
n_blades	number of blades
n_faces	number of faces

Acronyms

BC	boundary condition
CAD	computer aided design
CFD	computational fluid dynamics
FVM	finite volume method
LDV	laser Doppler velocimetry
LES	large eddy simulation
(L) GPL	(Lesser) General Public License
MRF	moving reference frame
(N) RMSD	(normalized) root-mean-square deviation
RDT	rapid distortion theory
RSM	Reynold stress equation model
SM	sliding mesh
STL	STereoLithography, "Standard Tessellation Language"

The steady-state MRF approach can be used to derive the flow field solely based on mixer and tank geometries, the viscosity of the fluid and propeller velocity (Bujalski et al., 2002; Deglon and Meyer, 2006; Sossa-Echeverria and Taghipour, 2015). There are two issues with this approach regarding the questions at hand: In the rotating frame the propeller is at rest. This implies that the position of the blades are static with respect to the tank, which is disadvantageous since many mobile agitators in the wine industry only have two blades. Hence, their position close to the tank wall will have a great influence on the solution. The other problem is, that this approach is not meant for transient simulations. A steady-state flow field may be calculated, but it is not possible to make predictions as to how long it will take until the steady-state flow field is established.

The SM approach is capable of simulating transient behavior and explicitly takes the rotation of the propeller into account (Bakker et al., 1997). Jaworski and Dudczak (1998) were among the first to use the SM technique with the standard k-ϵ turbulence model on stirred tank simulations. They showed adequate results for macromixing simulations in a Rushton turbine. For axial propellers, like the ones used primarily in the wine industry, Bakker et al. (1996) conducted laser Doppler velocimetry (LDV) experiments and validated multiple turbulence models for laminar and turbulent flow simulations using SM. It has to be noted, however, that most SM simulations in the literature have been conducted on very small tanks with comparatively large propellers and slow rotational speeds (for an overview see Joshi et al. (2011), Ochieng et al. (2009)).

In the wine industry, propellers typically rotate very fast with rotational speeds of more than 15 Hz and their size is small in comparison to the tank size. As a consequence, very small computational cells must be used in the proximity of the propeller to resolve the geometry. These cells are exposed to the highest velocities in the computational domain, which leads to small time steps and long computational times due to the Courant number restriction, Eq. (1). To ensure accuracy of the results and stability during processing, the Courant number should be restricted even in implicit simulations. Low numerical dissipation is expected when the product of the average velocity ($\tilde{v}$) and time step (Δt) is smaller than the average cell diameter (ΔI) (Ferziger et al., 1997).

$$c_r = \frac{\tilde{v}\Delta t}{\Delta I} \leqslant 1 \tag{1}$$

1.3. Goal of study and implementation of a new approach

To overcome the above mentioned problems, we developed a new approach using a time-varying, mapped, fixed-value boundary condition on the outside of the propeller zone (referenced from here on as ”transient BC" approach). Considering the high computational cost of SM, it has long been suggested to use the MRF approach to model a converged, time-averaged flow field and subsequently apply the SM technique to the rotating zone to model the tracer distribution (Jaworski et al., 2000). In our transient BC approach, we apply a similar idea where certain fields are time-dependently mapped from a precursor simulation using MRF and SM. To avoid the presumably very well mixed, but computationally demanding region around the propeller, this area is left blank in the new model and is no longer a part of the computational domain.

The transient BC approach can facilitate the use of CFD for large tank mixing, allow analyses on tank-mixer scenarios in the wine industry, and help to save resources by optimizing mixing times and processes. The goal of this study is to show that the method produces results comparable to the SM approach with a significant reduction in computational expense.

2. Materials and methods

2.1. Statement of the problem

The physical problem under investigation is the flow in a closed tank initiated by a mechanical mixer. Different CFD approaches of predicting the transient development of the flow field are analyzed. The fluid is considered incompressible and Newtonian.

2.2. Governing equations of the mathematical model

The governing equations solved for the flow field are the Navier-