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Numerical comparison of bubbling in a waste glass melter

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ABSTRACT

Radioactive tank waste is scheduled for vitrification at the Waste Treatment and Immobilization Plant (WTP) being constructed at the Hanford Site. Testing of the pilot-scale DuraMelter 1200 at the Vitreous State Laboratory at the Catholic University of America has demonstrated that bubbling increases the melt rate of the batch material, and as a result, melter throughput. Computational fluid dynamics (CFD) models of this pilot-scale waste glass melter are being developed to improve our understanding of the processes that occur within the melter to aid in process optimization and troubleshooting of the WTP melters. Unfortunately, model validation is complicated by the difficulty of obtaining suitable experimental data for operational melters due to the inaccessibility for direct observation and measurements of the high-temperature, opaque fluid through the water-jacketed, refractory-lined steel vessel. This study focuses on assessing the fidelity of the CFD models to accurately predict the bubbling behavior. Because of the paucity of experimental data at the resolution required for CFD validation, a code comparison was used to evaluate two common approaches for simulating flows of two immiscible Newtonian fluids on numerical grids and resolving multiphase interfaces. Here, the volume of fluid and level set methods are used to resolve the dynamically evolving interfaces between the molten glass and the air bubbles. To aid in the validation of the results of these codes, a comparison of the bubble behavior, growth, and frequency of bubble generation are presented and a grid convergence study is performed for the two approaches. The predictions from the two codes are within 6% for the average bubble radius of curvature within the bubble channels, within 2% for average terminal rise velocity of the bubbles, and within 4% for the area mean of the local maxima at the free surface. These parameters are of interest since they affect the convection within the melter and at the interface between the glass and batch layer. Ultimately, the results of this work can assist in confirming the predictive ability of waste glass melter models and provide a better understanding of the flow patterns within the WTP melters.

1. Introduction

At the Hanford Site in the state of Washington, more than 212 million liters of radioactive liquid waste is currently stored in underground tanks. This waste is the result of 45 years of defense plutonium production by the United States (U.S.) (Guillen and Beers, 2015). Currently, the tank waste is scheduled to undergo vitrification in large, steel melters being constructed at the Waste Treatment and Immobilization Plant (WTP). By mixing the waste with glass-forming additives, a stable borosilicate glass waste form is produced. Low-activity or high-level waste (HLW) forms will be stored in stainless steel containers or canisters for interim storage onsite or permanent repository disposal.

The Vitreous State Laboratory (VSL) at the Catholic University of America has tested vitrification systems at various scales using surrogate HLW formulations over the past several decades (Matlack et al., 2010). During these experiments, the melters were equipped with bubblers (Matlack et al., 2006, 2005; Kruger et al., 2013). From tests conducted with the pilot-scale DM1200 and other waste glass melters, it was concluded that the addition of bubblers into the system greatly enhances convective mixing and heat transfer, thereby increasing the rate of waste processed (Matlack et al., 2002; Hodges et al., 2012).

CFD models of the waste glass melter are useful to improve our understanding of the complex, interrelated processes occurring within the melter (Abboud and Guillen, 2016a,b; Abboud et al., 2016; Cambareri and Bolotnov, 2016). The behavior of bubbles rising in a room temperature viscous fluid has been characterized by numerous studies (Aybers and Tapucu, 1969; Raymond and Rosant, 2000; Snabre and Magnifotcham, 1998; Chen et al., 1999;

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Nomenclature

A	Area (m^2)
a	Radius of curvature (m)
c_p	specific heat (J/kg-K)
Cu	Courant number
C_θ	Model constant with the default value of 0.05
D	Bubble departure diameter (m)
Eo	Eötvös number
f	Resulting bubble radius of curvature
f_{RE}	Richardson extrapolated solution
f_d	Bubble departure frequency (s^{-1})
F_s	Safety factor
f_d	Bubble departure frequency
f	Exact solution
g	Gravitational acceleration (m/s^2)
g_p	Taylor series coefficient
h	Mesh resolution
H_ε	Heaviside function
N_f	Viscosity number
n	Normal vector
$O(h^{p+2})$	Leading error term
p	Order of accuracy
Q_e	Bubbler exit flowrate, l/min
R	Bubble radius of curvature (m)
r	Grid refinement factor
Re	Reynolds number
T	Stress tensor
u	Flow velocity vector
U_T	Terminal velocity (m/s)
V	Volume (m^3)
V_i	Specific fluid volume
v_g	reference frame velocity relative to the inertial laboratory frame
v	velocity in the stationary laboratory reference frame (absolute velocity)
We	Weber number

Greek letters

α_i	volume fraction
αc	Central volume fraction
αD	Downwind volume fraction
αu	Upwind volume fraction
$\Delta\rho$	Density difference between bubble and liquid (kg/m^3)
2ε	Interface thickness
ε	Discretization error
γ	Density ratio
κ	Interface curvature
μg	Gas viscosity (Pa-s)
μl	Liquid viscosity (Pa-s)
μ	Viscosity (Pa-s)
μgl	Viscosity ratio
ϕ	Distance away from the interface
ρ_i	Phasic density (kg/m^3)
ρg	Gas density (kg/m^3)
ρl	Liquid density (kg/m^3)
σ	Surface tension (mN/m)
s_{α_i}	phase-dependent volumetric source terms
θ	Angle between the surface normal and cell face normal
ξ_f	Normalized face value
ξ_c	Normalized face value in the vicinity of the cell center C

Simmons et al., 2015; Haberman and Morton, 1956; Golovin and Ivanov, 1971; Liu et al., 2015; Maxworthy et al., 1996; Lakehal et al., 2002; Chatzikyriakou et al., 2011; Clift et al., 1978; Guillen, 2016). The bubbles have a significant effect on the hydrodynamics and flow pattern. Multiphase solution frameworks are used to simulate the air injection into the molten glass phase. As the molten glass is much more viscous than water, large bubbles form, which require multiphase methods capable of resolving the interface between two immiscible fluids. Specifically, the volume of fluid (VOF) and level set (LS) methods are used in this work to capture the position of the interface between each phase (Hirt and Nichols, 1981; Sussman et al., 1994).

Due to the design of the melter, there is limited experimental data that can be used to validate the results of the CFD models. Validation of CFD predictions for large-scale, complex industrial equipment is much more challenging than well-controlled academic experiments conducted in a laboratory setting. The melter operates at high temperatures, contains opaque fluids and is constructed of water-jacketed, refractory-lined steel, all unfavorable conditions for the collection of the CFD quality validation data. In a previous study, numerical simulations of bubbling were validated against experimental data for air bubbling in highly viscous zinc bromide as a proxy for the waste glass (Abboud and Guillen, 2016a). In this paper, a code comparison using a recognized Code Comparison Principle outlined by Trucano et al. (2013) is implemented to assess the ability of two CFD codes to reliably characterize forced air bubbling in a highly viscous liquid. To ensure the fidelity of the simulation results, they must be verified through a grid convergence study and the comparison between the independent CFD models. This comparison is used to assist in the validation of the results from each simulation, ensuring that the most accurate representation of the bubbling is obtained. These simulations are part of a hierarchical validation methodology that segregates and simplifies the physical phenomena affecting the multiphase flow and heat transfer within a waste glass melter. The purpose of these simulations is to assess and validate the bubbling behavior isolated from other physics occurring in the melter. This tiered approach to model validation consists of a series of progressively more complex test cases designed to model the physics occurring in the full-scale system (Oberkampf and Trucano, 2000). Note that the multiphase methods used have a rich history of verification and validation for multiphase flow simulations (Rhee et al., 2005; Pan and Langberg, 2011; Akwa et al., 2012; Thomas et al., 2015; Nagrath et al., 2005; Bolotnov et al., 2011; Behafarid et al., 2015). A series of benchmark simulations devised to assess the fidelity of various interface tracking methods (ITMs) in various CFD codes, including STAR-CCM+, are discussed in Chatzikyriakou et al. (2011).

The aim of this research activity is to complete a direct comparison of CFD models of bubbling in a pilot-scale waste glass melter to increase confidence in the fidelity of the simulation methodology. The code comparison must also consider common errors that are made during solution verification, as noted by Trucano et al. (2013). Code verification to identify programming errors is typically performed by the software developer (Roy, 2005). These errors can include, but are not limited to, the assumption that the code solution is correct, using only qualitative comparisons, computing on only one mesh size, and showing results only where the code performs well (Trucano et al., 2013). This work addresses these issues by employing multiple meshes for a grid convergence study, using quantitative results alongside qualitative ones and delivering all relevant results, rather than a small subset of data where the comparisons are favorable. With these procedures, confidence in the reliability of the simulations is enhanced.