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A robust CFD model for freezing and melting in reservoir for Adblue (SCR) tanks

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Abstract

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1. Introduction

The modelling of melting and solidification (or thawing) is a challenging topic which had initially been studied extensively in the 80's and 90's for its application in metallurgical processes such as casting [1] in order to predict the crystal growth structure and the ensuing metallurgic properties. Since then, it has garnered continuous large interest for energy applications such as latent heat storage due to its various applicability in a large range of engineering fields [2, 3, 4, 5]. In this latter application, the interest has lied more in predicting accurately the melting or freezing rate and the overall heat storage instead of the precise position of the solid-liquid interface.

Other recent applications require a accurate prediction of the position of the melting and solidification interface. An example lies in the storage of AdBlue, a urea-water solution which is used for the Selective Catalytic Reduction (SCR) of the exhaust gas of diesel engines [6, 7]. The implementation of this technology, which has the potential to greatly reduce nitrogen oxides (NO_x) emissions, faces considerable challenges in colder regions of the world since AdBlue freezes and expands around -11C. This has two effect. First, the tanks must be able

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to handle freezing of the fluid without endangering the structure of the vessel, which could lead to leakage or worse, total breakage. Considering the complex shape that such reservoir can take, this requires an accurate prediction of the solidification front in order to prevent the occurence of liquid entrapment in solidified Adblue. Such entrapment leads to the generation of a high pressure zone which could distort or break components. Such predictions have to be carried out taking into account various factors which may alter the freezing dynamics, such as the parking angle of the vehicle. Secondly, the tank must house component that can thaw a sufficient amount of Adblue using minimal energy so that the system can operate even if the majority of the tank remain frozen. Thus, it is important to develop robust numerical models that can simulate freezing and thawing while predicting the position of the interface with great accuracy in order to ensure adequate design and operations of SCR components.

A second application lies in laser powder-bed fusion additive manufacturing. In this type of process, a laser is user to melt metal powder, creating a melted pool of liquid which then solidifies, ensuring buildup of the desired geometry [8, 9]. For such processes, accurate prediction of the solid-liquid interface as well as the flow dynamnics are critical.

From a physical and mathematical point of view, the modeling of phase changes is complex since they include sharp moving non-linear interfaces, an issue that may be exacerbated by the occurrence of natural convection .

When the flow is at high Rayleigh number, natural convection can have a considerable influence on the freezing or melting processes. We recall the definition of the Rayleigh number :

$$Ra = \frac{\rho^2 \beta g \left(T_w - T_s\right)}{k\mu} \tag{1}$$

with ρ the density of the fluid, β its linear coefficient of expansion, g the gravity, T_w the wall temperature, T_s the melting point temperature, k the thermal conductivity and μ the dynamic viscosity. Models for freezing and melting become inherently complex due to the coupling between the solid-liquid discontinuity, the natural convection and the non-linear variations of the physical properties of the material (such as the thermal conductivity) .Consequently, the velocity and the energy equation become tightly coupled. However, the phase change (i.e melting or solidification) occurs on a very slow time scale compared to the convective one. This seperation of time scale must be taken into account when designing numerical methods and, for instance, can render direct explicit approach prohibitively expensive due to the long physical time that must be simulated.

A large variety of numerical methods have been developed to tackle

In this work, we present three stabilized implicit finite element model for phase changes with natural convection. These model differ by the approach used to solve the energy conservation equation as well as to impose a no-slip boundary condition on the surface of the solidified material.

The first model uses a nodal temperature formulation as well as a hybrid enthalpy/temperature formulation at the integration points to take into account the phase change. This model is akin to a classical Eulerian approach for phase change, but the inclusion of stabilization in this present work makes it more robust and allows for a thinner mushy zone. In the second model, an hybrid nodal temperature-enthalpy formulation is used to increase the robustness of the implicit solver. These first two approaches impose the stasis of the fluid by using a viscous penalization of the momentum equation.

The third approach uses a conformal decomposition to reconstruct the solid-liquid interface within the elements. Thus an immersed boundary condition can be used to impose no-slip on the surface of the solidified material. This decomposition is also used for the energy equation in a nodal to ensure comformity.

The three approaches to resolve the phase change are first verified on the classical Stefan test case. The role of stabilization to improve the stability and robustness of the model is discussed. The influence of the model parameters on the stability and the accuracy of the model is established using mesh refinement analysis.

The accuracy of the strategies used to impose stasis are compared via order of convergence analysis.

The model is then validated by studying the melting of solified liquid in a cavity heated up by a vertical wall. Comparison with the literature shows that the models are able to reproduce melting front instabilities at high Rayleigh number and the relative accuracy of the models are compared. Finally, the thawing of a solid heated from below is studied and the formation of peculiar flow patterns is discussed. Future work possibilities deriving from this model, such the modeling of phase change of substances with different solid and liquid densities, are discussed as concluding remarks.

2. Model Formulation

3. Conclusion

4. Acknowledgements

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