Towards a robust implicit finite element formulation for solidification and melting processes with free surfaces

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ABSTRACT

The modelling of freezing and melting process is a difficult topic which has recently garnered increasing industrial interest. An example lies in the storage of AdBlue, an urea-water solution which is used for the Selective Catalytic Reduction (SCR) of the exhaust gas of diesel engines [1]. 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. Indeed, since AdBlue freezes around -11°C and expands upon freezing, the reservoirs storing the fluid must be adapted to the density change of the liquid which induce considerable stresses on the tank wall. The tank must also be adequately equipped to melt the frozen AdBlue as the engine is started. One additional hurdle in dealing with the freeze/thaw of urea solution is that the tank design involves quite often complex shapes as this component is designed using only the remaining available space once other components are integrated. Consequently, it becomes important to have potent numerical tools that may simulate the freezing and melting of AdBlue in reservoirs in order to assist in their design and to ensure adequate operation of the system [2].

From a physical and mathematical point of view, the modelling 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. Since the latter has a considerable influence on the freezing or melting processes, 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 density). Consequently, the velocity and the energy equation become tightly coupled. However, the solidification phenomena occurs on a very slow time scale compared to the convective one, which renders direct explicit approach prohibitively expensive due to the long physical time that must be simulated.

In this work, we present a novel implicit finite element model for phase changes with natural convection that takes into account the deforming free surface between the liquid and air. The model uses a hybrid enthalpy/temperature formulation for the liquid and solid phases while keeping track of the fluid-air interface using a Level Set approach. This allows for the simulation of phase changes on a static Eulerian mesh without requiring a specific treatment of the solid-fluid interface, while maintaining the capacity to simulate the thermal expansion due to the phase change.

The model is first validated on the Stefan test case. The influence of the model parameters on the stability and the accuracy of the model is established using mesh refinement analysis. The model is then used to study a classical melting and freezing problem in a two dimensional cavity, with and without the inclusion of the free surface. Comparison with the literature shows that the model is able to reproduce melting instabilities at high Rayleigh number. Finally, the model is used to study the solidification of AdBlue in a realistic reservoir. Future work possibilities deriving from this model, notably the inclusion of fluid-structure interaction, are discussed as concluding remarks.

[1] aus der Wiesche, S. (2007). Numerical heat transfer and thermal engineering of AdBlue (SCR) tanks for combustion engine emission reduction. Applied thermal engineering, 27(11), 1790-1798.

[2] Choi, B., & Woo, S. M. (2015). Numerical analysis of the optimum heating pipe to melt frozen urea-water-solution of a diesel urea-SCR system. Applied Thermal Engineering, 89, 860-870.