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Uncertainty Quantification of Phase Transition Problems with an Injection Boundary

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Abstract. We develop an enthalpy-based modeling and computational framework to quantify uncertainty in Stefan problems with an injection boundary. Inspired by airfoil icing studies, we consider a system featuring an injection boundary inducing domain changes and a free boundary separating phases, resulting in two types of moving boundaries. Our proposed enthalpy-based formulation seamlessly integrates thermal diffusion across the domain with energy fluxes at the boundaries, addressing a modified injection condition for boundary movement. Uncertainty then stems from random variations in the injection boundary. The primary focus of our Uncertainty Quantification (UQ) centers on investigating the effects of uncertainty on free boundary propagation. Through mapping to a reference domain, we derive an enthalpy-based numerical scheme tailored to the transformed coordinate system, facilitating a simple and efficient simulation. Numerical and UQ studies in one and two dimensions validate the proposed model and the extended enthalpy method. They offer intriguing insights into ice accretion and other multiphysics processes involving phase transitions.

AMS subject classifications: 35R60, 80A22, 35R35, 65M06, 35B30

Key words: Uncertainty quantification, phase transition, injection boundary, enthalpy method.

1 Introduction and motivation

Phase transition problems play a pivotal role in understanding fundamental physical processes like melting and solidification. These phenomena have substantial ramifica-

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tions across various scientific disciplines, including materials science and aerospace engineering (cf. [1,22,26]). Specifically, these problems involve the intricate dynamics of heat transfer occurring at the interfaces between different phases of materials. This heat transfer, in turn, induces the motion of these phase boundaries. Quantifying and predicting such interplay between heat diffusion and interface movement constitute the fundamental essence of phase transition problems. And these problems are also commonly referred to as the Stefan problems.

Phase transition phenomena, coupled with material injection, are also ubiquitous problems in various scientific and engineering problems. One illustrative example motivating research in this field is the challenge posed by ice formation on aircraft airfoils (see, cf. [6,8,16–20,22,30]). When aircraft operate at high altitudes, they encounter water droplets present in clouds and mist, which can adhere to the aircraft's surfaces, leading to ice formation. Accurately predicting the type and location of ice accumulation is essential for ensuring flight safety and stability. Consequently, this necessity has spurred extensive research into phase transition problems involving injection boundaries, accompanied by corresponding numerical simulations (see, cf. [8,17,20]).

Moreover, quantifying uncertainties in such phase transition problems with injection boundaries has substantial value. Uncertainty stems from influential uncertain factors affecting the dynamics and subsequent dynamic performance. Conducting uncertainty quantification can shed light on the extent to which uncertain conditions impact the problem and foster a deeper understanding of the underlying mechanisms. However, this remains challenging partially due to the complex interactions between the moving phase interface and injection dynamics in high-dimension. To enable reliable uncertainty analysis, specialized modeling, and computational techniques are required to account for these coupled physics.

In this work, we aim to develop an integrated framework combining UQ techniques with phase transition modeling and simulations tailored for the phase transition problems with an injection boundary. The enthalpy-based model we considered in two-dimension in this paper is

$$\rho c\frac{\partial U}{\partial t}=k\Delta U,\quad (y,x,t)\in(0,1)\times(0,S(y,t))\times(0,\infty), \tag{1.1}$$

$$\rho c\frac{\partial U}{\partial t}=k\Delta U,\quad (y,x,t)\in(0,1)\times(S(y,t),L(t))\times(0,\infty), \tag{1.2}$$

$$U(y,S(y,t),t)=T_m, \tag{1.3}$$

$$\rho L_h v_n(y,t)(t)=k[\nabla U\cdot\boldsymbol{n}](y,S(y,t),t), \tag{1.4}$$

$$k\frac{\partial U}{\partial x}(y,L(t),t)+\frac{dL(t)}{dt}H(y,L(t)-,t)=\eta(y,t)\frac{dL(t)}{dt}. \tag{1.5}$$

The spatial domain representing the region occupied by the materials in both phases is $(y,x)\in[0,1]\times[0,L(t)]$, where y is the horizontal position and x is the vertical position. In this context, U represents the temperature and H represents the enthalpy (or the total heat energy, to be introduced in Eq. (2.1) with ρ,c denoting the density and specific heat