International Journal of Heat and Mass Transfer 227 (2024) 125603

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Comment on "Numerical study with OpenFOAM on heat conduction problems in heterogeneous media" by K. Zhang, C.-A. Wang, J.-Y. Tan, International Journal of Heat and Mass Transfer, Vol. 124 (2018) 1156–1162

J. Bohacek [a,*], K. Mraz [a], J. Hvozda [a], F. Lang [a], E. Karimi-Sibaki [b,c], A. Vakhrushev [b,c], A. Kharicha [b,c]

[a] Heat Transfer and Fluid Flow Laboratory, Faculty of Mechanical Engineering, Brno University of Technology, 61669 Brno, Czech Republic
[b] Christian-Doppler Lab for Metallurgical Applications of Magnetohydrodynamics, Montanuniversitaet of Leoben, Franz-Josef-Str. 18, 8700 Leoben, Austria
[c] Chair of Simulation and Modeling of Metallurgical Processes, Montanuniversitaet Leoben, Franz-Josef-Str. 18, A-8700 Leoben, Austria

ARTICLE INFO

Keywords
Heat conduction
Diffusion equation
Heterogeneous media
Anisotropic material
Thermal diffusivity
OpenFOAM

ABSTRACT

In the paper "Numerical study with OpenFOAM on heat conduction problems in heterogeneous media" by K. Zhang, C.-A. Wang, J.-Y. Tan, International Journal of Heat and Mass Transfer, Vol. 124 (2018) 1156–1162 the authors modify laplacianFoam from open-source CFD package OpenFOAM® to solve heat conduction problems in heterogeneous media by changing the diffusion coefficient from a constant value to a scalar field. Their paper clearly demonstrates a fundamental, overlooked, and common mistake in rearranging the heat conduction equation, which cannot be replaced with the temperature diffusion equation. In this comment, we provide clear evidence through mathematical derivations and numerical examples calculated in OpenFOAM®.

1. Remarks

The well-known heat conduction equation, also known as the energy equation, is defined by the first law of thermodynamics and Fourier's law as follows:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla\cdot(\lambda \nabla T), \tag{1}$$

in which T is temperature (K), and t is time (s). Density ρ (kgm^{-3}), specific heat c_p (Jkg^{-1} K^{-1}) and thermal conductivity λ (Wm^{-1} K^{-1}) are thermal properties of a substance or material, which conducts the heat.

Heat conduction problems are often modeled using the diffusion equation, which is given by:

$$\frac{\partial T}{\partial t} - \nabla\cdot(\alpha \nabla T) = 0, \tag{2}$$

in which α is the thermal diffusion coefficient (m^2 s^{-1}), defined as $\alpha = \lambda/(\rho c_p)$.

In this work, we comment on the paper "Numerical study with OpenFOAM on heat conduction problems in heterogeneous media" [1], in which Zhang et al. incorrectly handle the fundamental process of conductive heat transfer.

Zhang et al. reused *laplacianFoam* from the popular open-source CFD package OpenFOAM® [2]. The solver *laplacianFoam* solves Eq. (2) while considering $\alpha = const$. Zhang et al. changed the declaration of α from a constant value to a scalar field and claimed the modified *laplacianFoam* suitable for numerical modeling of heat conduction problems in heterogeneous material by setting different values of α for each phase. This is incorrect unless a clear definition of (rather rare) heterogeneous material is provided or correct boundary conditions are ensured at the interface between the phases through a source term added to Eq. (2).

When dealing with heat conduction problems in heterogeneous material, which may consist of two or more different phases, a proper boundary condition (BC) must be set at the interface between the phases (Fig. 1). This BC of conjugate heat transfer must ensure the continuity of the normal heat flux and temperature at the interface and can be written as follows:

$$\boldsymbol{n}\cdot\lambda_1\nabla T_1 = \boldsymbol{n}\cdot\lambda_2\nabla T_2, \tag{3}$$

* Corresponding author.
E-mail address: jan.bohacek@vut.cz (J. Bohacek).

https://doi.org/10.1016/j.ijheatmasstransfer.2024.125603
Received 26 March 2024; Received in revised form 18 April 2024; Accepted 19 April 2024

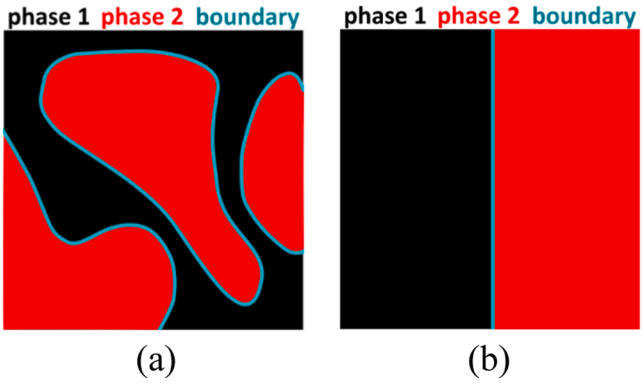

Fig. 1. A schematic representation of a heterogeneous material consisting of phase 1 (ρ_1, c_{p1} and λ_1) and phase 2 (ρ_2, c_{p2} and λ_2); a two-layer plate adapted from Ref. [1] by Zhang et al.

$$T_1 = T_2, \tag{4}$$

in which $\boldsymbol{n}$ is the normal vector to the interface and the subscripts 1 a 2 denote respectively the phase 1 and the phase 2, as shown in Fig. 1.

There are two contrasting, but correct, approaches to the numerical solution of heat conduction in heterogeneous materials. In the first, Eqs. (1) and (2) is considered separately in each phase and the problem is linked together by Eqs. (3) and (4). In the second, Eq. (1) is considered with the scalar fields of ρ, c_p and λ mapped over the whole space domain. The interface conditions are satisfied implicitly, although the heat flux and temperature at the interface are determined using interpolation schemes that take values from both phases. The former excels in accuracy, while the latter excels in the calculation speed and dealing with complex or boundary misaligned meshes.

In Ref. [1], Zhang et al. adopted the second approach. However, he considered the diffusion equation, Eq. (2), instead of the energy equation, Eq. (1). Regarding Eq. (2), recall that the thermal diffusion coefficient α measures the ability of a material to conduct thermal energy *relative* to its ability to store thermal energy. Although Eqs. (1) and (2), are both written in a conservative form, in the latter the heat flux is conserved based on α and not λ. Hence, the interface boundary condition is only satisfied, when the ratio α_1/α_2 matches the ratio λ_1/λ_2. Note that it only happens when the heat capacitance $\rho c_p = const$.

It is straightforward to prove the abovementioned statement by substituting α with $\lambda/(\rho c_p)$ in Eq. (2) to recover the terms of Eq. (1). After rearranging the terms, we arrive at:

$$\frac{\partial T}{\partial t} = \nabla\cdot(\alpha\nabla T) - \nabla\left(\frac{1}{\rho c_p}\right)\cdot(\lambda\nabla T) \tag{5}$$

Inside each phase, Eq. (5) is indeed identical to Eq. (2), because the source (or sink) term becomes zero. However, Eq. (2) is incomplete at the boundary between the phases because of the missing source term.

The following exemplary cases will further manifest the difference in results between Eq. (1) and inappropriate Eq. (2). For that purpose, the two-layer plate geometry is adopted from Ref. [1], shown also in Fig. 1 (b). Like Zhang et al., we also set α_1 and α_2 to each layer and expose the plate to Dirichlet boundary conditions on the sides and zero heat flux at the top and the bottom.

In the first case (Fig. 2(a)), air and steel are selected to represent the layers. Air and steel are materials commonly encountered in simulations of metallurgical processes. As the temperature drops, the casting shrinks, and the air gap is formed near the mold [3]. Air convection is neglected here. When the energy equation, Eq. (1), or the diffusion equation with the source term, Eq. (5), is used, the temperature gradient in steel is expectedly negligibly small compared to the gradient in air. When Eq. (2) is employed, unphysical results are obtained. The incorrect single-sloped temperature profile is caused by very similar α_1 and α_2, yet very different ρ_1, c_{p1}, λ_1 and ρ_2, c_{p2}, λ_2.

In the second case (Fig. 2(b)), the materials are selected such that $\alpha_1 \neq \alpha_2$, but $\lambda_1 = \lambda_2$. This condition is practically held, e.g., with the oak wood and the ethylene-glycol. Eq. (1) provides a correct temperature profile. Eq. (2) leads again to unphysical results.

In conclusion, considering spatially varying thermal diffusivity α within a heterogeneous material and solving Eq. (2) leads to unphysical results.

CRediT authorship contribution statement

J. Bohacek: Writing – review & editing, Writing – original draft, Conceptualization. **K. Mraz:** Software. **J. Hvozda:** Formal analysis. **F. Lang:** Visualization. **E. Karimi-Sibaki:** Writing – review & editing, Writing – original draft. **A. Vakhrushev:** Software, Methodology. **A. Kharicha:** Project administration, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

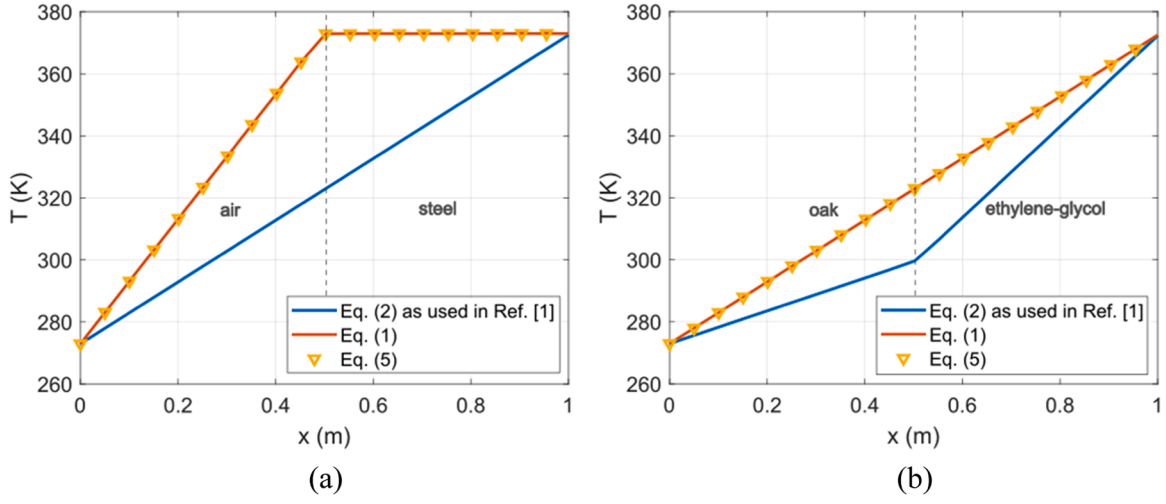

Fig. 2. Steady-state temperature profiles across the two-layer plate calculated for (a) $\alpha_1 = \alpha_2$ and (b) $\lambda_1 = \lambda_2$ using Eq. (2) reproduced from Ref. [1], Eq. (1) and Eq. (5) solved in the present study in OpenFOAM®.

Data availability

Data will be made available on request.

Acknowledgements

The paper presented has been supported by the internal grant of the Brno University of Technology Focused on Specific Research and Development no. FSI-S-23-8254. The authors acknowledge the financial support by the Austrian Federal Ministry of Economy, Family and Youth and the National Foundation for Research, Technology and Development within the Framework of the Christian Doppler Laboratory for Metallurgical Applications of Magnetohydrodynamics. Computational resources were supplied by the project "e-Infrastruktura CZ" (e-INFRA CZ LM2018140) and supported by the Ministry of Education, Youth and Sports of the Czech Republic. Computational resources were provided by the ELIXIR-CZ project (LM2018131), part of the international ELIXIR infrastructure.

References

[1] K. Zhang, C.-A. Wang, J.-Y. Tan, Numerical study with OpenFOAM on heat conduction problems in heterogeneous media, Int. J. Heat Mass Transf. 124 (2018) 1156–1162, https://doi.org/10.1016/j.ijheatmasstransfer.2018.04.038.

[2] H.G. Weller, G. Tabor, H. Jasak, C. Fureby, A tensorial approach to computational continuum mechanics using object-oriented techniques, Comput. Phys. 12 (1998) 620, https://doi.org/10.1063/1.168744.

[3] J. Bohacek, A. Kharicha, A. Ludwig, M. Wu, E. Karimi-Sibaki, Heat transfer coefficient at cast-mold interface during centrifugal casting: calculation of air gap, Metall. Mater. Trans. B 49 (2018) 1421–1433, https://doi.org/10.1007/s11663-018-1220-0.