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Benchmarking Numerical Freeze/Thaw Models

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Abstract

The modeling of freezing and thawing of water in porous media is an area of increasing interest. Examples include the modeling of permafrost degradation due to climate change, geotechnical applications in tunneling, and borehole heat exchanger performance in cold regions. Different code implementations have been developed and an interest has arisen in benchmarking different codes with analytical solutions, experiments, and numerical results. The name for this benchmark consortium is INTERFROST. Benchmark results are shown for a 1D analytical solution and two different 2D set-ups. All compared codes exhibit a similar behavior.

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Keywords: groundwater; permafrost; soil freezing; analytical solution; numerical model

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1. Introduction

The modeling of freezing and thawing of water in porous media is a research topic of increasing interest, and for which very different applications exist [1]. For instance, the modeling of permafrost regression with respect to climate change issues is one area, while others include geotechnical applications in tunneling or geothermal applications for borehole heat exchangers which operate at temperatures below the freezing point.

The modeling of these processes requires the solution of a coupled non-linear system of partial differential equations for flow and heat transport in space and time.

Nomenclature

S_s	specific storage (m^{-1})
ρ	density (kg m^{-3})
c	specific heat capacity (J kg^{-1} K^{-1})
T	temperature (°C)
λ	thermal conductivity (W m^{-1} K^{-1})
∇	Laplace operator
H	heat sources (W m^{-3})
Q	fluid sources (s^{-1})
K	hydraulic conductivity (m s^{-1})
h	head (m)
t	time (s)
S_w	water saturation (-)
L	latent heat of fusion for bulk medium (J m^{-3})
q	Darcy velocity (m s^{-1})
Indexes	
g	bulk value
f	fluid phase

The groundwater flow equation and coupled heat transport equation are shown in Eqs. (1) and (2), respectively [2,3,4,5]:

$$S_s \frac{\partial h}{\partial t} = \nabla \cdot (\mathbf{K} \nabla h) + Q \tag{1}$$

$$(\rho c)_g \frac{\partial T}{\partial t} + L \frac{\partial S_w}{\partial t} = \nabla \cdot (\boldsymbol{\lambda} \nabla T - \rho_f c_f \mathbf{q} T) + H \tag{2}$$

with

$$\mathbf{q} = -\mathbf{K} \nabla h \tag{3}$$

Different code implementations have been developed in the past [1], although analytical solutions to compare these alternative implementations only exist for simple cases. Consequently, an interest has arisen in benchmarking different codes with analytical solutions, experiments, and purely numerical results, similar to the long-standing DECOVALEX collaboration project [6] for coupled numerical models and the more recent “Geothermal Code Comparison” [7] activities.

INTERFROST is a new freeze-thaw benchmark consortium that has been initiated to address this need. All details for the benchmarks shown can be found at https://wiki.lsce.ipsl.fr/interfrost/. At present, in total 13 different codes are included in this benchmark project [8]. Here only a comparison is shown between the results of Cast3M [9], SMOKER [10], SUTRA-ICE [3] and FEFLOW [11] which is coupled with a newly programmed plug-in [5,12].

2. Benchmarks

2.1. T1: Lunardini/Osterkamp

This case is a purely thermal simulation of the frost penetration into a porous soil body. The formulations of the analytical solution are based on the original work of Stefan [13]. In contrast to the freezing process of bulk water, water in porous media freezes gradually over a temperature range. This freezing interval is defined as the difference in the minimum temperature for which the pore water is fully liquid and the maximum temperature for which the pore water is fully frozen except for the residual liquid water content. The width of the freezing interval depends on many factors such as the salt content, overburden pressure, and grain sizes.

Lunardini [14] developed an analytical solution to calculate the location of the freezing interval in a semi-infinite domain with three zones: unfrozen, partially frozen (or 'mushy'), and fully frozen (Fig. 1). Fig. 2 shows the location of the temperature front where water first begins to freeze as compared to the results from the numerical models. The analytical and numerical results are in a good agreement.

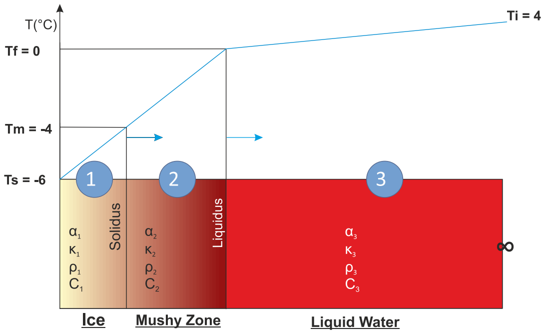

Fig. 1. Three-zone model (ice, mushy zone, liquid water) with a schematic temperature profile. Herein, freezing occurs between -4 and 0°C [3, 15].

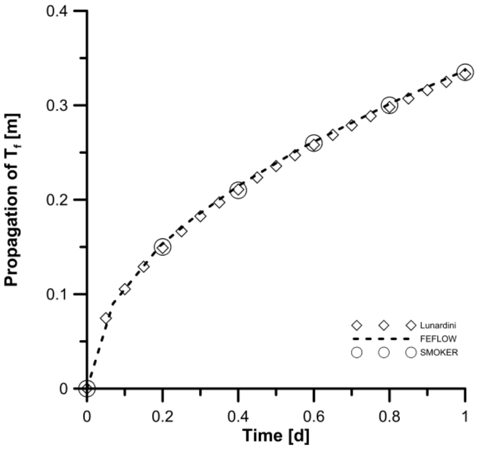

Fig. 2. Comparison of the results for the T1 Lunardini solution with two numerical codes. Results for SUTRA, which also matches this solution, are presented in [3].

2.2. TH2: Melting of a Frozen Inclusion

This artificial test case simulates the thermo-hydraulically (TH) coupled thawing process of a frozen inclusion in a porous medium. As such, calculations have highly transient and differential characteristics - direct analytical solutions do not exist. Thermal and hydraulic boundary conditions induce coupled heat and water flow that influences the thawing rate (Figs. 3 and 4). At temperatures below the freezing point of the pore water, the hydraulic conductivity of the soil is reduced via an exponential impedance factor. During the thawing process the hydraulic conductivity increases continuously until the intrinsic value for unfrozen conditions is attained. Due to the convective heat transport, the system is highly transient. In order to verify the TH coupling, four different hydraulic gradients are imposed (0, 3, 9 and 15 %). The TH coupled process induces a cold temperature plume which either expands due to thermal conduction around the initial frozen inclusion for the zero-gradient case, or expands and migrates downgradient due to advection and conduction for the non-zero gradient cases.

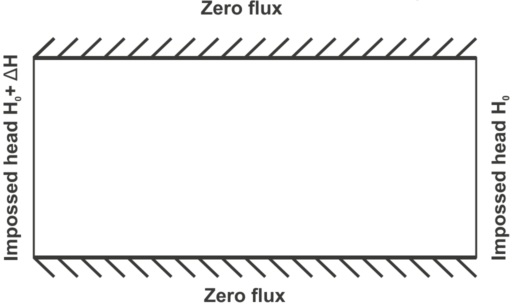

Fig. 3. Schematic of the test model (TH2) and hydraulic boundary conditions [15].

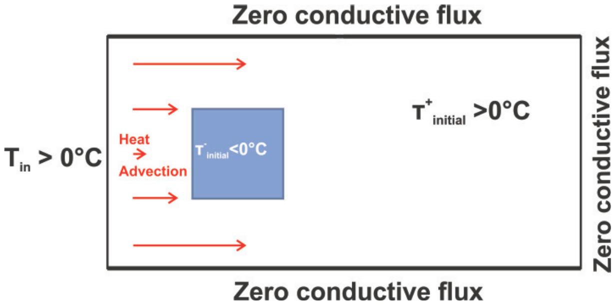

Fig. 4. Thermal boundary conditions of the test model TH2 [15].

This benchmark problem was modeled by the four above-mentioned software codes for coupled thermo-hydraulic heat transport (Cast3M, SUTRA-ICE, FEFLOW, and SMOKER). Each code is capable of accommodating the thermal and hydraulic effects of freezing and melting processes. For comparing results, three time-steps were defined (t = 0.2, 0.3, and 0.4 days). The results are subject to be verified by experimental data and further comparison to other numerical solutions. A subset of the results is shown in Fig. 5 and Fig. 6.

Table 1. TH2 benchmark details.

	Cast3M	**SUTRA-ICE**	**SMOKER**	**FEFLOW-FTM**
Mesh Size	31609 Nodes, 31104 Elements	20301 Nodes, 20000 Elements	60802 Nodes, 30000 Elements	16394 Nodes, 30740 Elements
Element Type	Quadrilateral	Quadrilateral	Rectangular prisms	Triangles

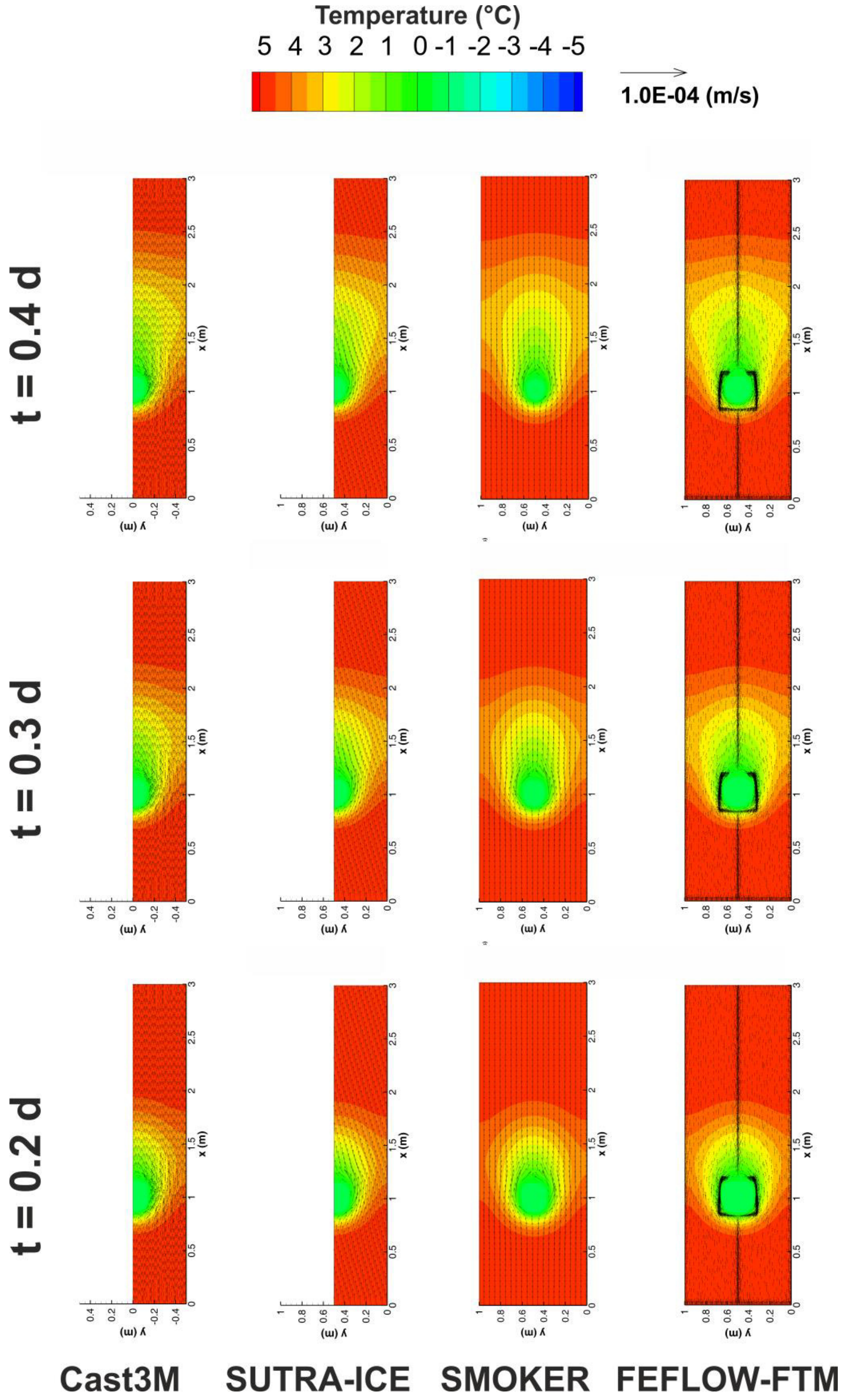

Fig. 5. Results of the TH2 benchmark. Evolution of temperature and flow rates (i = 3 %). Due to the problems symmetry the Cast3M and SUTRA-ICE solutions reflect only one half of the domain.

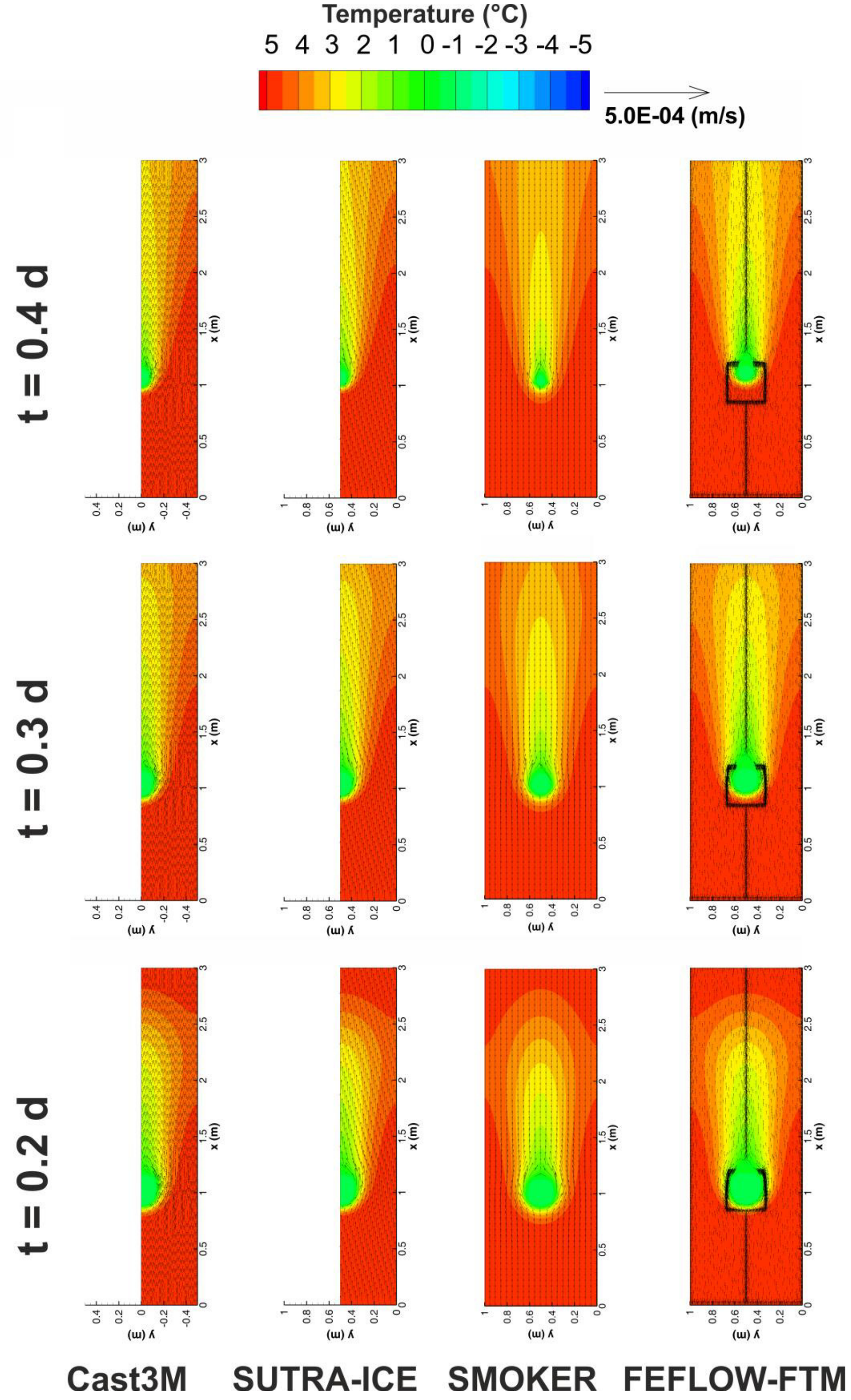

Fig. 6. Results of the TH2 benchmark. Evolution of temperature and flow rates (i = 9 %). Due to the problems symmetry the Cast3M and SUTRA-ICE solutions reflect only one half of the domain.

2.3. TH3: Talik Opening/Closure

Talik regions (anomalous unfrozen zones) provide important conduits for groundwater flow within continuous permafrost regions. The benchmark TH3 simulates concurrent freezing and thawing processes in an idealized domain. The general configuration is shown in Fig. 7. The opening or closure of the talik is influenced by the temperature boundary conditions and the rate of groundwater flow through the domain. The boundary conditions of this test case are chosen such that both the opening and the closure are simulated. The configuration for the hydraulic boundary conditions is similar to the TH2 benchmark (Fig. 3).

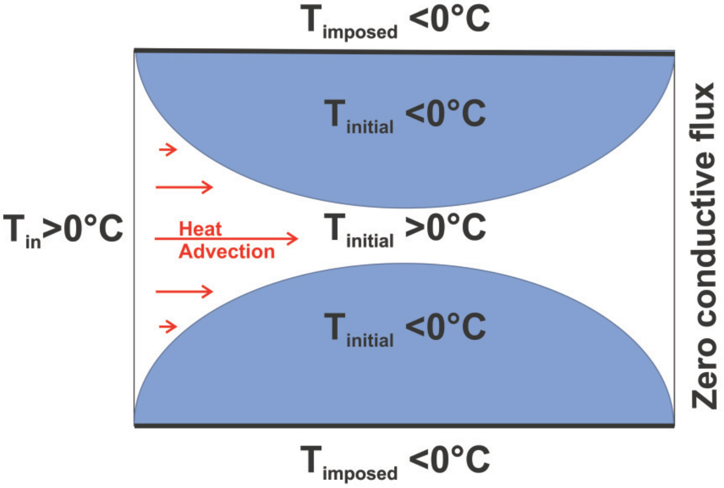

Fig. 7. TH3: Opening/Closure of a talik in benchmark TH3 [15].

Again, the benchmark is simulated for imposed head gradients of 0, 3, 6, 9 and 15 %. Fig. 8 and Fig. 9 show a comparison of the Cast3M, SUTRA-ICE, FEFLOW-FTM, and SMOKER results at different times based on hydraulic gradient of 3 % and 9 %. All of the numerical codes calculate the opening or closing process well. The FEFLOW result is computed with an automatic mesh refinement (AMR) within the freezing zone between zero and minus one degrees Celsius. Within this range the mesh density is increased automatically to improve the accuracy of the numerical solution

Table 2. TH3 benchmark details.

	Cast3M	**SUTRA-ICE**	**SMOKER**	**FEFLOW-FTM**
Mesh Size	8848 Nodes, 17272 Elements	45451 Nodes, 45000 Elements	20402 Nodes, 10000 Elements	Initially: 966 Nodes, 1788 Elements; later on automatically refined
Element Type	Triangles	Quadrilateral	Rectangular prisms	Triangles

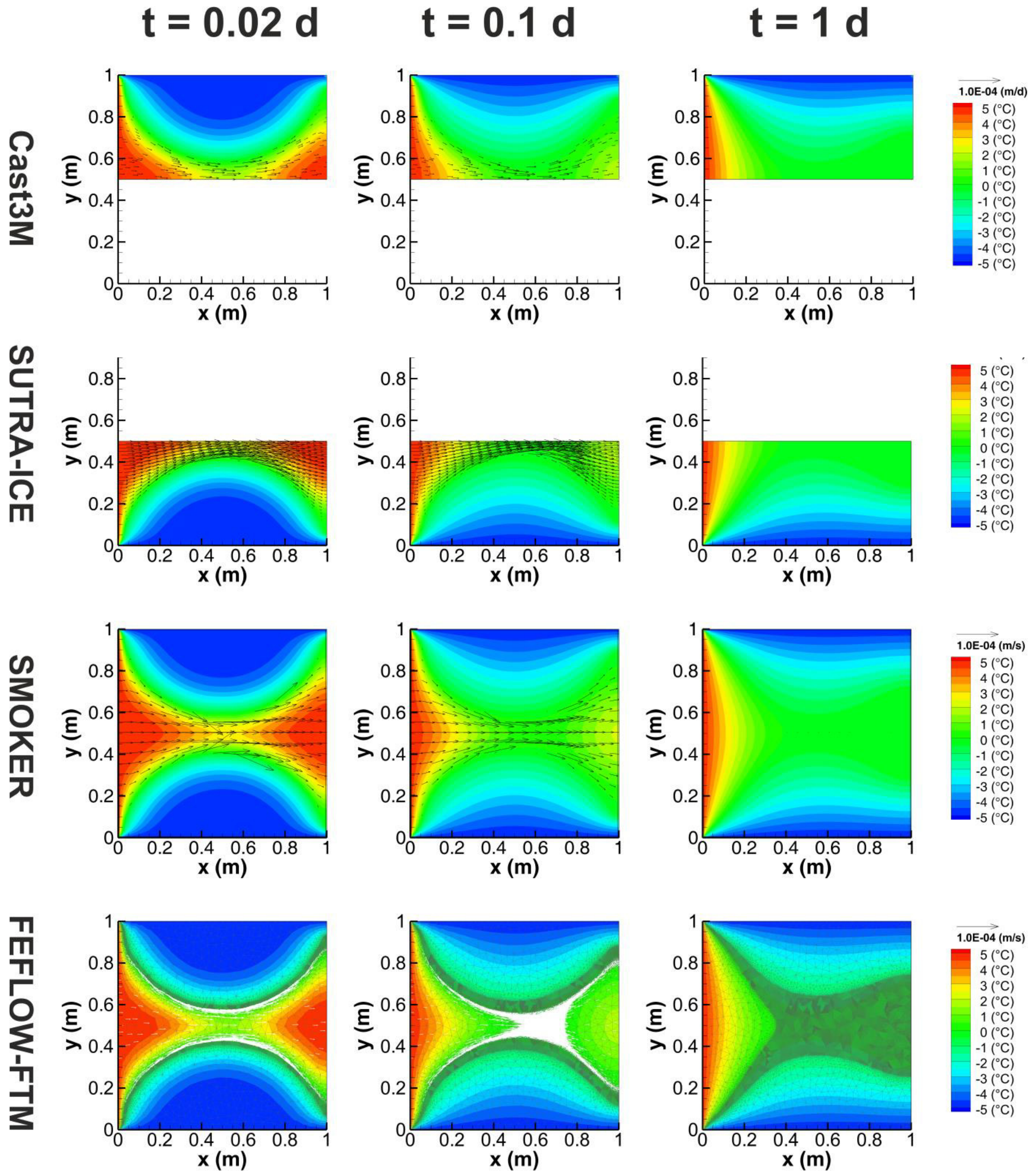

Fig. 8. Results of the TH3 benchmark. Evolution of temperature and flow rates (i = 3 %). Due to the problems symmetry the Cast3M and SUTRA-ICE solutions reflect only one half of the domain.

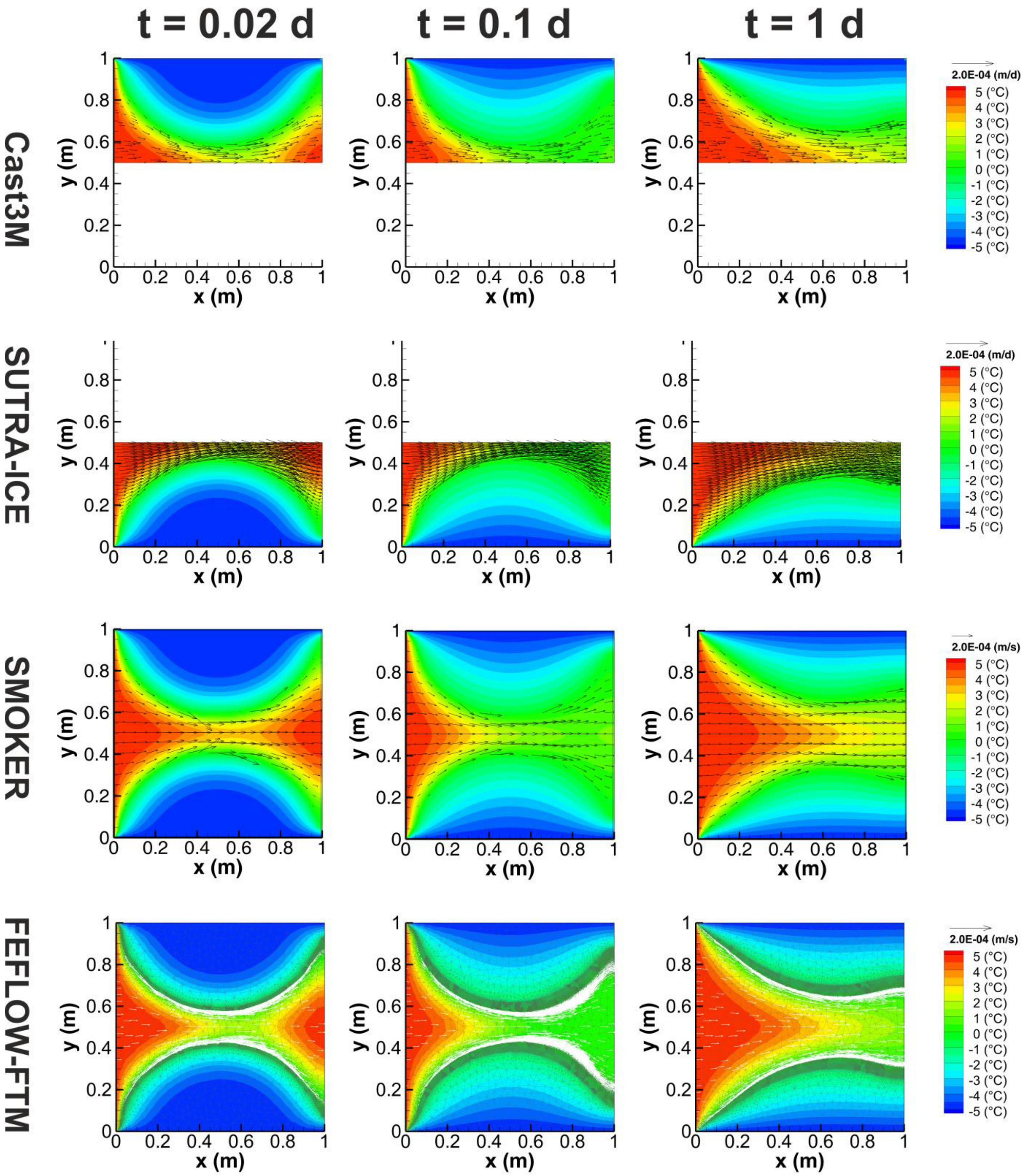

Fig. 9. Results of the TH3 benchmark. Evolution of temperature and flow rates (i = 9 %). Due to the problems symmetry the Cast3M and SUTRA-ICE solutions reflect only one half of the domain.

4. Discussion

The benchmark results exhibit a good qualitative similarity between the different codes. For a quantitative evaluation, specific performance measurements have been developed (see https://wiki.lsce.ipsl.fr/interfrost/). The results are scheduled for publication in early 2016. Further elaboration on the test cases and a comparison to experimental data are anticipated.

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