A benchmark for the validation of solidification modelling algorithms

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Abstract. This work presents two three-dimensional solidification models, which were solved by several commercial solvers (MAGMASOFT, FLOW-3D, ProCAST, WinCast, ANSYS, and OpenFOAM). Surprisingly, the results show noticeable differences. The results are analyzed similar to a round-robin test procedure to obtain reference values for temperatures and their uncertainties at selected positions in the model. The first model is similar to an adiabatic calorimeter with an aluminum alloy solidifying in a copper block. For this model, an analytical solution for the overall temperature at steady state can be calculated. The second model implements additional heat transfer boundary conditions at outer faces. The geometry of the models, the initial and boundary conditions as well as the material properties are kept as simple as possible but, nevertheless, close to a realistic solidification situation. The gained temperature results can be used to validate self-written solidification solvers and check the accuracy of commercial solidification programs.

1. Introduction

During a recent research project, significant differences in the results of numerical simulations using different commercial simulation programs were noticed by the authors. Especially the release of heat at solidification of an alloy varied considerably with the selected programs. This fact led to a literature search for a benchmark model configuration describing a simple solidification problem. Whereas different benchmark studies are found for relatively complex simulations of fluid flow (e.g. [1-4]), little is published for the simple diffusive transport of heat including the change of state. While analytical solutions are available for one-dimensional semi-infinite configurations [5], no numerical solutions for a heat conduction problem with release of heat of fusion have been found.

Two simple models, close to a realistic solidification situation, were set up to check several commercial solvers similar to a round-robin test with regard to their accuracy to compute the temperature distribution. The first model is a solidifying aluminum cube in an isolated cube-shaped copper mold; this configuration is in principle an adiabatic calorimeter. This has the advantage that the final common temperature of the aluminum and copper after an infinite time can be analytically calculated. The second model is the same geometrical configuration, but with heat transfer at two of the outer walls in order to check the influence of boundary conditions.

The models were computed with the following software programs: MAGMASOFT version 5.2 [6], FLOW-3D version 10.1 [7], ProCAST version 2013.0 [8], WinCast version [9], ANSYS Workbench version 14.5 [10], and OpenFOAM (in a customized version) [11]. For the following, the software...
programs are – according to the rules of a round-robin test – anonymized and given arbitrary numbers from 1 to 6.

Based on the results of the inter-comparison, the support of the software manufacturer of these two programs with noticeably deviating results was contacted. One of the programs was updated immediately (within some days) for a software bug; the second program needed a much tighter convergence for the release of heat of fusion compared to the standard adjustment, resulting in smaller time steps and longer computation time.

2. Models

Figure 1 shows a sketch of the geometry of the two models consisting of a mold with an overall dimension of 50 mm x 50 mm x 50 mm; a second cube of melt measuring 20 mm x 20 mm x 20 mm is placed in the center. At zero time the mold has a temperature of $T_{\text{mold}}=200^\circ\text{C}$ and the melt $T_{\text{melt}}=700^\circ\text{C}$. The heat transfer coefficient at the faces between the two materials is constant at a value of $HTC_{\text{internal}}=100 \text{ W m}^{-2} \text{ K}^{-1}$. Three measuring points for temperature (P1, P2, and P3), marked as green dots, are defined in order to compare the simulation results among the different software programs. A cooling time of 1200 s is specified to ensure a temperature very close to equilibrium for both metals at the end of the simulation.

The first model has adiabatic boundary conditions at all outer walls. In this case, the equilibrium temperature of the melt and mold after an infinite time can be analytically calculated. The temperature measurement point P1 is in the center of the aluminum melt with the coordinates $x=25$ mm, $y=25$ mm, $z=25$ mm and the point P2 is located in a corner of the copper mold with the coordinates $x=48.5$ mm, $y=48.5$ mm, $z=1.5$ mm.

The second model has heat transfer boundary conditions at two opposite outer walls ($x_{\text{min}}$ and $x_{\text{max}}$ in fig. 1). A heat transfer coefficient of 2000 W m$^{-2}$ K$^{-1}$ to the surrounding ($HTC_{\text{external}}$), which is kept at 20°C, is defined, while the other four walls are kept adiabatic. One temperature measurement point is again P1 in the center, the second point P3 is on the horizontal line of symmetry at the coordinates $x=42.5$ mm, $y=25$ mm, $z=25$ mm.

![Figure 1. Geometry of the simulation models.](image)

Table 1 and 2 show the thermophysical properties of the materials used. Intentionally, the properties are close to copper and aluminum alloy, but simplified. The values of density $\rho$, specific heat capacity $c_p$ and thermal conductivity $\lambda$ are kept constant in the entire temperature range. The fraction solid is a linear function of temperature between liquidus and solidus temperature.
Table 1. Thermophysical properties of the mold material

| Property           | Value     |
|--------------------|-----------|
| Density $\rho_{\text{mold}}$ | 8900 kg m$^{-3}$ |
| Specific heat $c_{p,\text{mold}}$ | 380 J kg$^{-1}$ K$^{-1}$ |
| Thermal conductivity $\lambda_{\text{mold}}$ | 320 W m$^{-2}$ K$^{-1}$ |

Table 2. Thermophysical properties of the melt material

| Property           | Value     |
|--------------------|-----------|
| Density $\rho_{\text{melt}}$ | 2700 kg m$^{-3}$ |
| Specific heat $c_{p,\text{melt}}$ | 1000 J kg$^{-1}$ K$^{-1}$ |
| Thermal conductivity $\lambda_{\text{melt}}$ | 150 W m$^{-2}$ K$^{-1}$ |
| Liquidus temperature $T_{\text{liquidus}}$ | 638°C |
| Solidus temperature $T_{\text{solidus}}$ | 520°C |
| Latent heat of fusion $L_{\text{fusion}}$ | 364 826 J kg$^{-1}$ (in addition to specific heat) |

3. Analytical solution for the adiabatic model
Comparing the enthalpies in the initial state ($T_{\text{mold}} = 200^\circ$C and $T_{\text{melt}} = 700^\circ$C) and in complete equilibrium state leads to an equilibrium temperature $T_{\text{equilibrium}}$:

$$T_{\text{equilibrium}} = \frac{V_{\text{mold}}\rho_{\text{mold}}c_{p,\text{mold}}T_{\text{mold}} + V_{\text{melt}}\rho_{\text{melt}}c_{p,\text{melt}}T_{\text{melt}} + L_{\text{fusion}}}{V_{\text{mold}}\rho_{\text{mold}}c_{p,\text{mold}} + V_{\text{melt}}\rho_{\text{melt}}c_{p,\text{melt}}},$$

where $V_{\text{mold}}$ is the volume of the mold, $V_{\text{melt}}$ is the volume of the melt. The equilibrium temperature of the adiabatic model results in $T_{\text{equilibrium}} = 244.7652^\circ$C.

4. Numerical solutions
The energy conservation equation in combination with Fourier’s law of heat transport under consideration of the release of heat leads to the equation for the change of temperature $T$ with time $t$

$$\frac{\partial}{\partial t}(\rho c_p T) = \nabla (\lambda \nabla T) + \rho L_{\text{fusion}} f_{\text{solid}}(T) \frac{\partial T}{\partial t},$$

where $\rho$ is density, $c_p$ is heat capacity, $\lambda$ is thermal conductivity, $L_{\text{fusion}}$ is heat of fusion, and $f_{\text{solid}}$ is the fraction of solid. Some of the used programs implement the release of heat of fusion by a modified heat capacity function.

This equation was numerically approximated by all used software programs. To achieve a realistic accuracy of the results similar to a “typical” software user, default software parameters (e. g. convergence criterions) were used as far as possible for the calculations. In relation to the relative simple model, the meshes were extremely fine. The temperatures at the defined positions in the models are recorded as a function of time for the inter-comparison.

Figure 2 shows the temperatures at point P1 and point P2 as a function of time for the adiabatic model; fig. 3 shows temperatures at point P1 and P3 for the model with external heat transfer. These results have been obtained by one of the commercial solvers.
Figure 2. Temperature as a function of time at two measuring points of the adiabatic model.

Figure 3. Temperature as a function of time at two measuring points of the model with external heat transfer.
5. Results and comparison

The temperature results as function of time at the “virtual thermocouple” points of the individual simulation results were fitted to be able to compare the results of the individual simulation programs at exactly the same instants of time. For the case of available temperature data close to the selected instant, the two neighboring points were fitted by a linear function. For wider gaps, the data in the liquid range, the solidification interval, and the solid range were fitted according to the equation:

\[ T = a + be^{-ct} \]  

(3)

where \( a, b, \) and \( c \) are constants. The deviation of the fitted data from the simulated temperatures is very small (in the Milli-Kelvin range) except close to zero time and in the vicinity of the beginning and the ending of solidification, where the temperature traces show characteristic kinks. The regions of noticeable deviations were omitted. Tables 3 and 4 show the results of the simulated temperatures of the adiabatic model at selected times at point P1 and P2, as well as the arithmetic mean and the standard deviation.

Table 3. Adiabatic model: Temperatures in the center of the melt (point P1) at selected times

| Time (s) | 1 (°C) | 2 (°C) | 3 (°C) | 4 (°C) | 5 (°C) | 6 (°C) | Arithmetic mean (°C) | Standard deviation (°C) |
|----------|--------|--------|--------|--------|--------|--------|----------------------|-------------------------|
| 6        | 669.65 | 669.46 | 669.23 | 669.34 | 669.45 | 669.75 | 669.43               | 0.16                    |
| 30       | 618.41 | 618.81 | 619.50 | 617.72 | 618.92 | 619.44 | 618.67               | 0.66                    |
| 60       | 586.73 | 587.05 | 588.18 | 585.98 | 586.92 | 587.70 | 586.97               | 0.79                    |
| 120      | 532.05 | 532.27 | 533.74 | 531.30 | 531.78 | 532.92 | 532.23               | 0.92                    |
| 170      | 426.40 | 426.29 | 431.26 | 423.88 | 424.73 | 428.77 | 426.51               | 2.86                    |
| 300      | 284.88 | 284.58 | 286.55 | 283.77 | 284.33 | 286.70 | 284.82               | 1.05                    |
| 600      | 245.90 | 245.97 | 246.08 | 245.95 | 246.19 | 246.65 | 246.02               | 0.12                    |
| 1200     | 244.67 | 244.77 | 244.73 | 244.91 | 245.02 | 245.04 | 244.82*              | 0.14                    |

*Exact result: \( T_{\text{equilibrium}} = 244.77°C \)

Table 4. Adiabatic model: Temperatures at the corner of the mold (point P2) at selected times

| Time (s) | 1 (°C) | 2 (°C) | 3 (°C) | 4 (°C) | 5 (°C) | 6 (°C) | Arithmetic mean (°C) | Standard deviation (°C) |
|----------|--------|--------|--------|--------|--------|--------|----------------------|-------------------------|
| 6        | 201.40 | 201.41 | 201.39 | 201.44 | 201.43 | 201.41 | 201.41               | 0.02                    |
| 30       | 207.65 | 207.67 | 207.58 | 207.75 | 207.76 | 207.66 | 207.68               | 0.08                    |
| 60       | 214.72 | 214.77 | 214.59 | 214.95 | 214.93 | 214.75 | 214.79               | 0.15                    |
| 120      | 226.93 | 227.00 | 226.71 | 227.28 | 227.29 | 226.99 | 227.04               | 0.24                    |
| 170      | 234.64 | 234.75 | 234.48 | 234.99 | 235.05 | 234.77 | 234.78               | 0.24                    |
| 300      | 242.45 | 242.57 | 242.46 | 242.74 | 242.83 | 242.62 | 242.61               | 0.17                    |
| 600      | 244.60 | 244.70 | 244.67 | 244.85 | 244.95 | 244.87 | 244.75               | 0.14                    |
| 1200     | 244.67 | 244.77 | 244.72 | 244.90 | 245.02 | 245.05 | 244.81*              | 0.14                    |

*Exact result: \( T_{\text{equilibrium}} = 244.77°C \)

Tables 5 and 6 show the results of the simulated temperatures of the second model with external heat transfer at selected times at point P1 and P3, the arithmetic mean of the temperatures and the standard deviation.
### Table 5. Model with external heat transfer: Temperatures at the center of the melt (point P1) at selected times

| Time (s) | Temperature results of simulation program number | Arithmetic mean (°C) | Standard deviation (°C) |
|----------|-----------------------------------------------|----------------------|------------------------|
|          | 1  | 2     | 3     | 4     | 5     | 6*    |                       |                       |
| 6        | 668.95 | 668.86 | 668.36 | 668.73 | 669.46 | 668.75 | 0.23                  |
| 30       | 613.44 | 615.13 | 615.47 | 615.11 | 617.83 | 614.86 | 0.81                  |
| 60       | 572.93 | 574.45 | 575.78 | 574.43 | 574.09 | 583.61 | 1.02                  |
| 120      | 424.79 | 427.11 | 434.27 | 426.71 | 424.48 | 520.20 | 3.97                  |
| 170      | 260.10 | 260.74 | 266.65 | 260.35 | 259.01 | 346.86 | 261.37                |
| 300      | 81.32  | 81.04  | 83.67  | 80.08  | 140.85 | 81.32  | 1.40                  |
| 600      | 22.61  | 22.56  | 22.80  | 22.28  | 22.52  | 36.48  | 22.55                 |

*Results excluded from mean value and standard deviation.

### Table 6. Model with external heat transfer: Temperatures at the center of the melt (point P1) at selected times

| Time (s) | Temperature results of simulation program number | Arithmetic mean (°C) | Standard deviation (°C) |
|----------|-----------------------------------------------|----------------------|------------------------|
|          | 1  | 2     | 3     | 4     | 5     | 6*    |                       |                       |
| 6        | 175.37 | 175.08 | 175.25 | 174.97 | 175.22 | 189.45 | 175.18                |
| 30       | 113.26 | 112.60 | 112.66 | 111.94 | 112.99 | 166.90 | 112.69                |
| 60       | 72.25  | 71.64  | 71.61  | 71.26  | 72.04  | 143.92 | 71.76                 |
| 120      | 41.30  | 41.06  | 41.06  | 40.94  | 41.25  | 110.40 | 41.12                 |
| 170      | 31.47  | 31.39  | 31.46  | 31.34  | 31.45  | 89.76  | 31.42                 |
| 300      | 22.69  | 22.68  | 22.77  | 22.62  | 22.68  | 53.32  | 22.69                 |
| 600      | 20.11  | 20.11  | 20.13  | 20.10  | 20.11  | 25.67  | 20.11                 |

*Results excluded from mean value and standard deviation.

Tables 7 shows the results of the simulated times ($t_{\text{liqidus}}$ and $t_{\text{solidus}}$) to reach the characteristic kinks at start and end of solidification ($T_{\text{liqidus}}$ and $T_{\text{solidus}}$) of both models at point P1.

### Table 7. Time from start to the characteristic kinks at $T_{\text{liqidus}}$ and $T_{\text{solidus}}$ (see fig. 2 and 3) in the center of the melt (point P1)

| Time results of simulation program number | Adiabatic model | Model with external heat transfer |
|------------------------------------------|-----------------|----------------------------------|
|                                          | 1 (s) | 2 (s) | 3 (s) | 4 (s) | 5 (s) | 6 (s) | 1 (s) | 2 (s) | 3 (s) | 4 (s) | 5 (s) | 6 (s) |
| $t_{\text{liqidus}}$                      | 12.35 | 12.21 | 12.33 | 12.68 | 12.21 | 12.00 | 12.30 | 0.21 |
| $t_{\text{solidus}}$                      | 134.12 | 134.01 | 135.88 | 133.02 | 133.56 | 135.26 | 134.31 | 0.98 |
|                                          | 12.01 | 11.61 | 11.79 | 11.77 | 11.51 | 12.22* | 11.74 | 0.17 |
|                                          | 99.84 | 100.11 | 101.57 | 100.26 | 99.72 | 120.00* | 100.30 | 0.66 |

*Results excluded from mean value and standard deviation.
6. Conclusions
Two simple heat transfer models describing diffusive heat transport and solidification were set up to check several commercial software solvers similar to a round-robin test to check their accuracy to compute temperature distributions. According to the rules of a round-robin test, no judgement of the quality or accuracy of the included solvers is given. Five of six solvers gave similar results with differences in the range of up to several degrees Celsius. One of them had been bug-fixed, the results of the fixed version are included, the original results have been omitted. The sixth solver deviates quite significantly when applying external heat transfer, the reason for this was not unveiled by the software manufacturer.

Following conclusions can be drawn:

- Commercial solvers can have (rarely, but it is happening) software bugs influencing the results even of simple solidification models. This could be due to frequent version changes.
- Differences between commercial solvers are in the range of up to several degrees Celsius, especially after the end of solidification. This could be due to the numerical treatment of the release of the heat of fusion in correlation to the computing speed optimization.
- For the model with external heat transfer, one of the programs was removed from the calculation of arithmetic mean and standard deviation due to a significant discrepancy.
- The models can be employed to validate self-written solidification solvers and check the accuracy of commercial solidification programs.

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