Numerical validation of the SNOW python package (version 1.0)

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Abstract

The authors validated the simulation outcome of the SNOW python package with the originally developed model in MATLAB and found an excellent agreement among the programs, for all relevant types of heat transfer and cooling protocols studied. Both the original MATLAB codes and the python package are available free of charge online. We will provide a more general description of the modeling framework in a publication in the future.

1 Validation

1.1 Methods

In order to compare the simulation outcomes between the two programs, we carried out a number of case studies. These case studies aim at testing all functionalities of the modeling framework. This comprises studies of all heat transfer types, of the cooling protocol, and of controlled nucleation. If not noted otherwise, the standard values of the snowfall package are used.

We base the comparison on the characteristic quantities of freezing, measuring the difference in the simulated distributions of the nucleation temperature and of the nucleation times among the simulations.

If not noted otherwise, the following model parameters were used: 1 mL of 5 wt.% sucrose solution, 49 vials on the shelf, 5000 repetitions, time step of 2 s, cooling rate of 0.5 $\mathrm{K min^{-1}}$ with initial temperature of 20°C and final temperature of -50°C.

1.2 Heat transfer validation

We carried out four studies to validate the heat transfer aspect of the simulations. The simulation results are summarized in figure 1 for the nucleation temperatures and in figure 2 for the nucleation times. In all four scenarios, the constant part of the heat transfer coefficient with the shelf was set to $k_{\mathrm{sh},0} = 20\ \frac{\mathrm{W}}{\mathrm{m^2K}}$. In scenario (a), all other heat transfer coefficients are set to zero. In scenarios (b) to (d), one additional heat transfer coefficient assumes a non-zero value each as illustrated in the figures 1 and 2. Please note that for scenario (d), in order to set $s_{\mathrm{sh}} = 2\ \frac{\mathrm{W}}{\mathrm{m^2K}}$, a value of $s\dot{}sigma\dot{}rel$ = 0.1 was used in the python package, which uses a relative definition of this quantity with respect to the overall shelf heat transfer coefficient. The MATLAB code, on the other hand, uses an absolute definition.

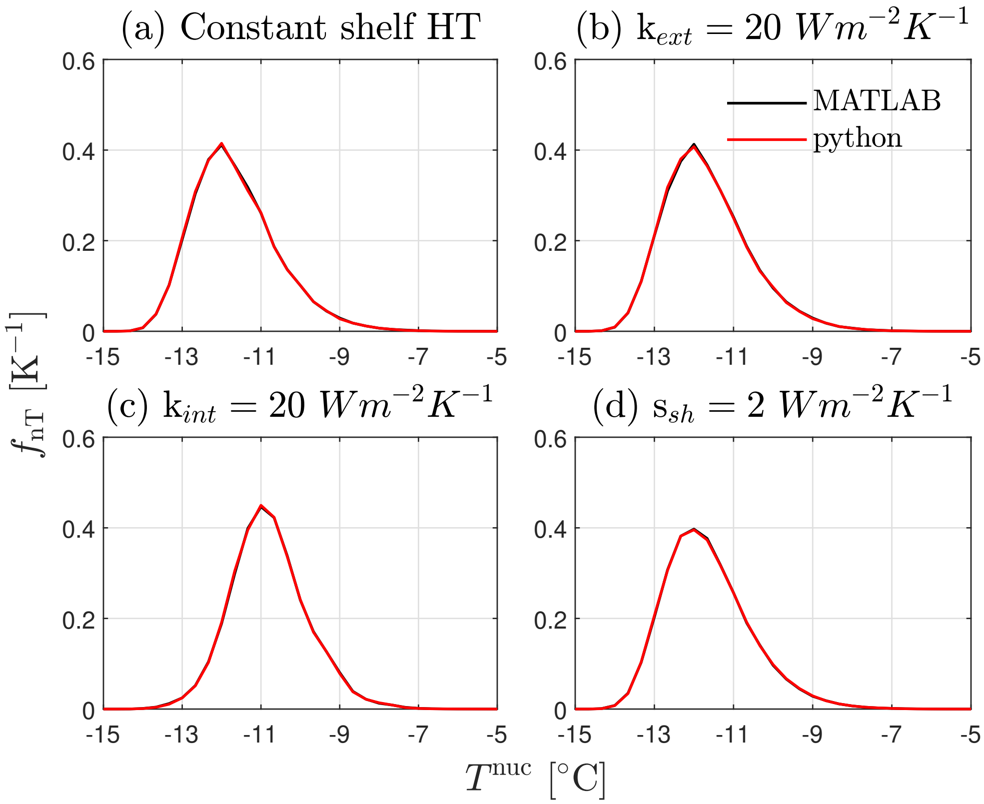

Figure 1: Validation of the simulated nucleation temperatures for four heat transfer scenarios: (a) Only constant heat transfer with the shelf, (b) constant shelf heat transfer and external heat transfer, (c) constant shelf heat transfer and internal heat transfer, (d) variable shelf heat transfer

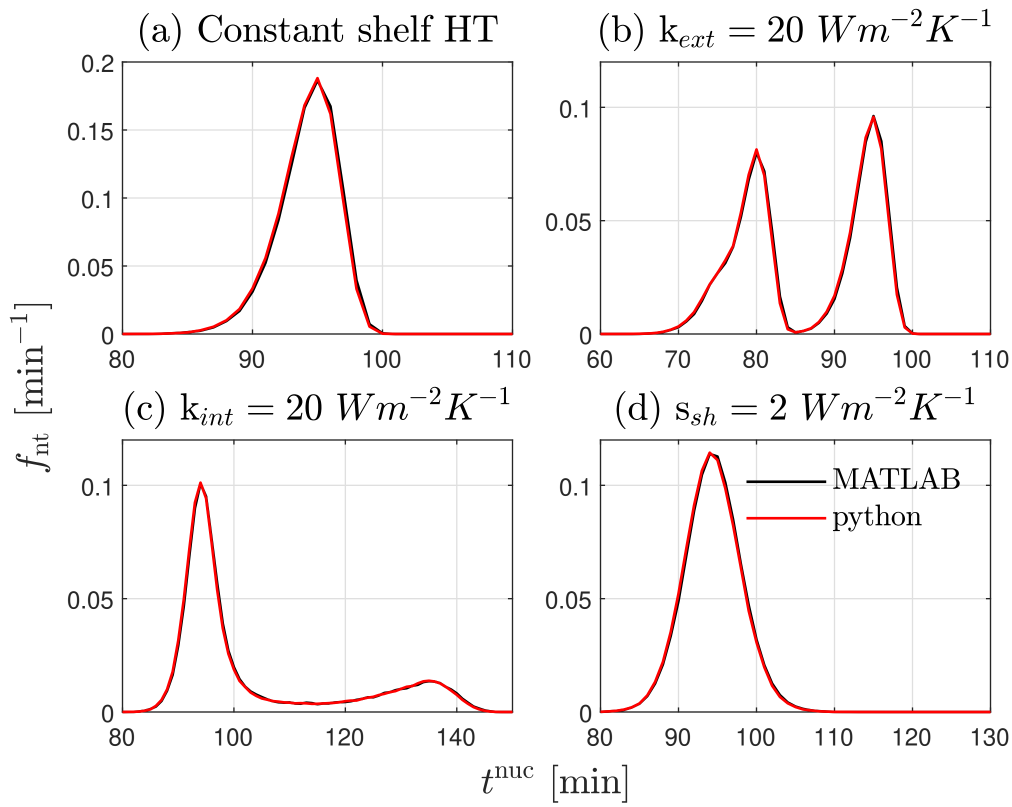

Figure 2: Validation of the simulated nucleation temperatures for four heat transfer scenarios: (a) Only constant heat transfer with the shelf, (b) constant shelf heat transfer and external heat transfer, (c) constant shelf heat transfer and internal heat transfer, (d) variable shelf heat transfer

For all four scenarios the agreement between the simulations in MATLAB and python is excellent with respect to both the distributions of nucleation temperatures and of nucleation times. A similar agreement was observed for the solidification times (not shown here).

1.3 Cooling protocol validation

To investigate how the simulation outcomes behave for complex cooling protocols, we studied two scenarios. Scenario (a) comprises an unsuccessful ad-nucleation holding step at -10°C for 540 min, as shown in figure 3. Scenario (b) comprises a process involving a pre-nucleation holding step at -5°C for 180 min, where nucleation is induced at the end of the hold. The characteristic quantities for this scenario are presented in figure 4.

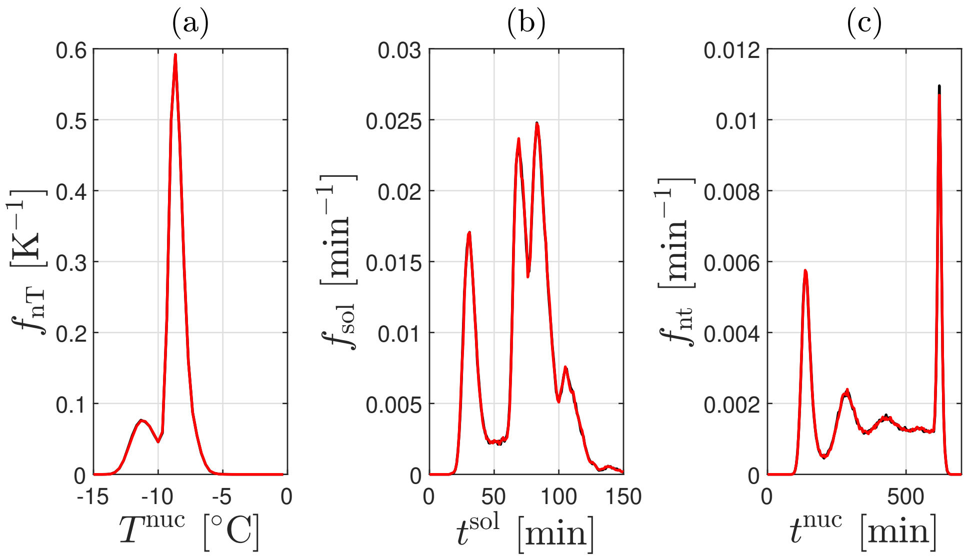

Figure 3: Validation of the simulated characteristic quantities among python (red) and MATLAB (black) codes for a complex cooling protocol comprising an ad-nucleation holding step. (a) Nucleation temperature distribution, (b) solidification time distribution, (c) nucleation time distribution.

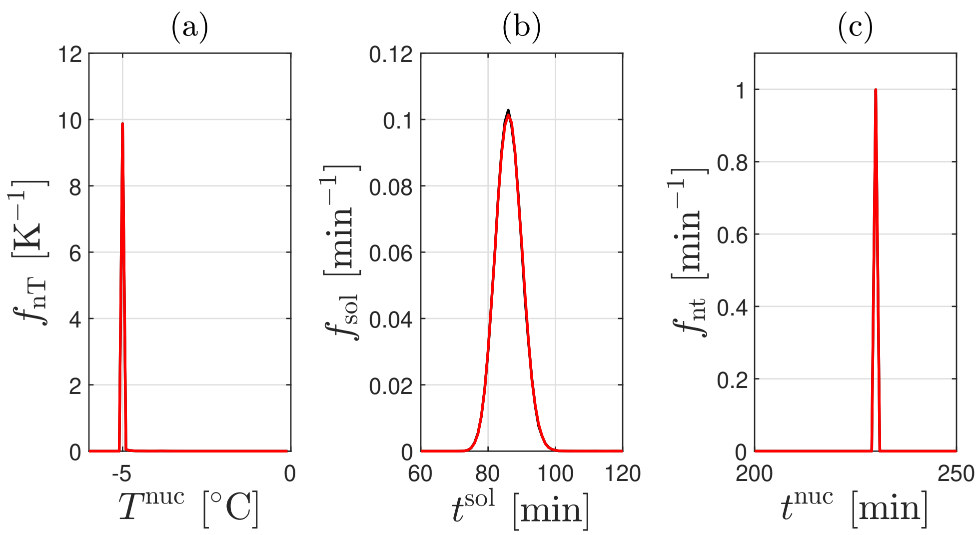

Figure 4: Validation of the simulated characteristic quantities among python (red) and MATLAB (black) codes for a complex cooling protocol comprising controlled nucleation at the end of a pre-nucleation holding step. (a) Nucleation temperature distribution, (b) solidification time distribution, (c) nucleation time distribution.

We again observe an excellent agreement between the two simulations in both scenarios. This confirms that the simulations even agree in the case of a complex cooling protocol (scenario (a)) and of controlled nucleation (scenario (b)), thus in all use cases that were originally considered when developing the MATLAB version.

1.4 Conclusion

During this validation study, we could not find any mismatch in the simulations between the MATLAB and python programs. We thus will use primarily the python version in the future due to its wider accessibility and recommend potential users to do so as well.