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## Background and Basics

- Temperatures influence biological processes in different ways. The reaction rate increases with temperature up to a certain level and then drops again. Above a limit temperature, biological molecules are denatured

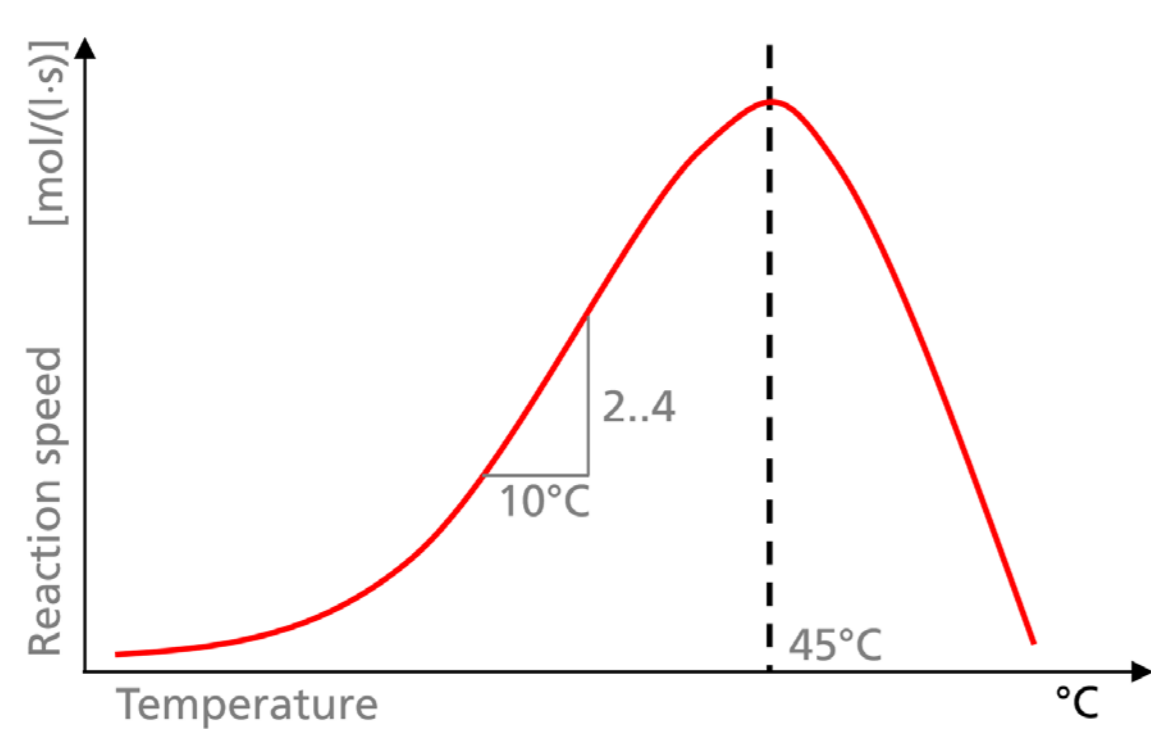


Figure 1: Reaction rate depending on temperature

- In most cases a liquid handling system contains temperature controlled devices, that emit heat. Usually, the temperature in a liquid handling systems is a result of the heat output of all devices
- For process safety, it is therefore necessary to monitor and control the temperatures precisely
- Narrow temperature windows are prescribed in regulatory environments

## Basics of heat transfer modeling

- Grey-Box approach
- Lumped-Capacitance model
- FDM methods for 3D visualisation
- Heat transfer & convection equations

## Setup

- A combination of temperature controlled devices from Inheco (CPAC, ODTC and ThermoshakeAC ) are used to cool and heat biological samples
- These devices are running inside a Tecan Fluent® Automation Workstation using the DreamPrep® NGS configuration
- To measure the temperatures on the devices and in the Tecan Fluent® Automation Workstation, a sensor system was set up to monitor a variety of relevant measurement points

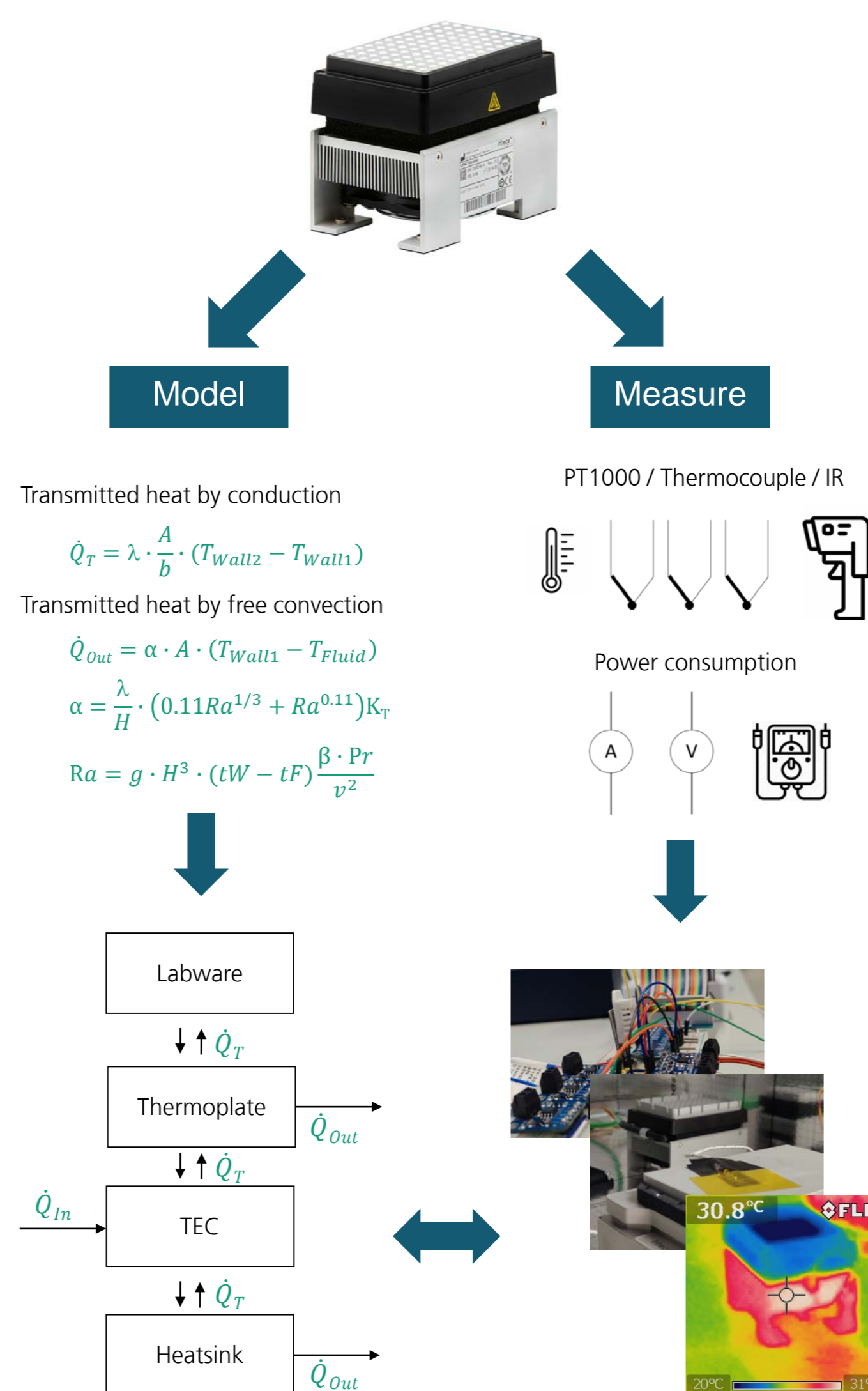


Figure 2: Modeling process based on heat transfer equations and measured data used for validation

## Procedure

- Examination of the devices and their operating principle (e.g. Peltier Elements)
- Setting up the differential equations (ODEs) for the device models
- Parameterisation of the device models based on physical properties of the devices (material, mass, etc.)
- Simulation of the temperature behavior of the device models based on their power consumption as input parameters
- Validation of the device models through comparison of measurement data from the real devices with simulated data
- Creation of a configurable simulation framework combining the device models in a liquid handler environment
- Adaption of the overall simulation framework to simulate temperature behavior using process parameters, like process time, lid state, target temperature for each device individually, as inputs

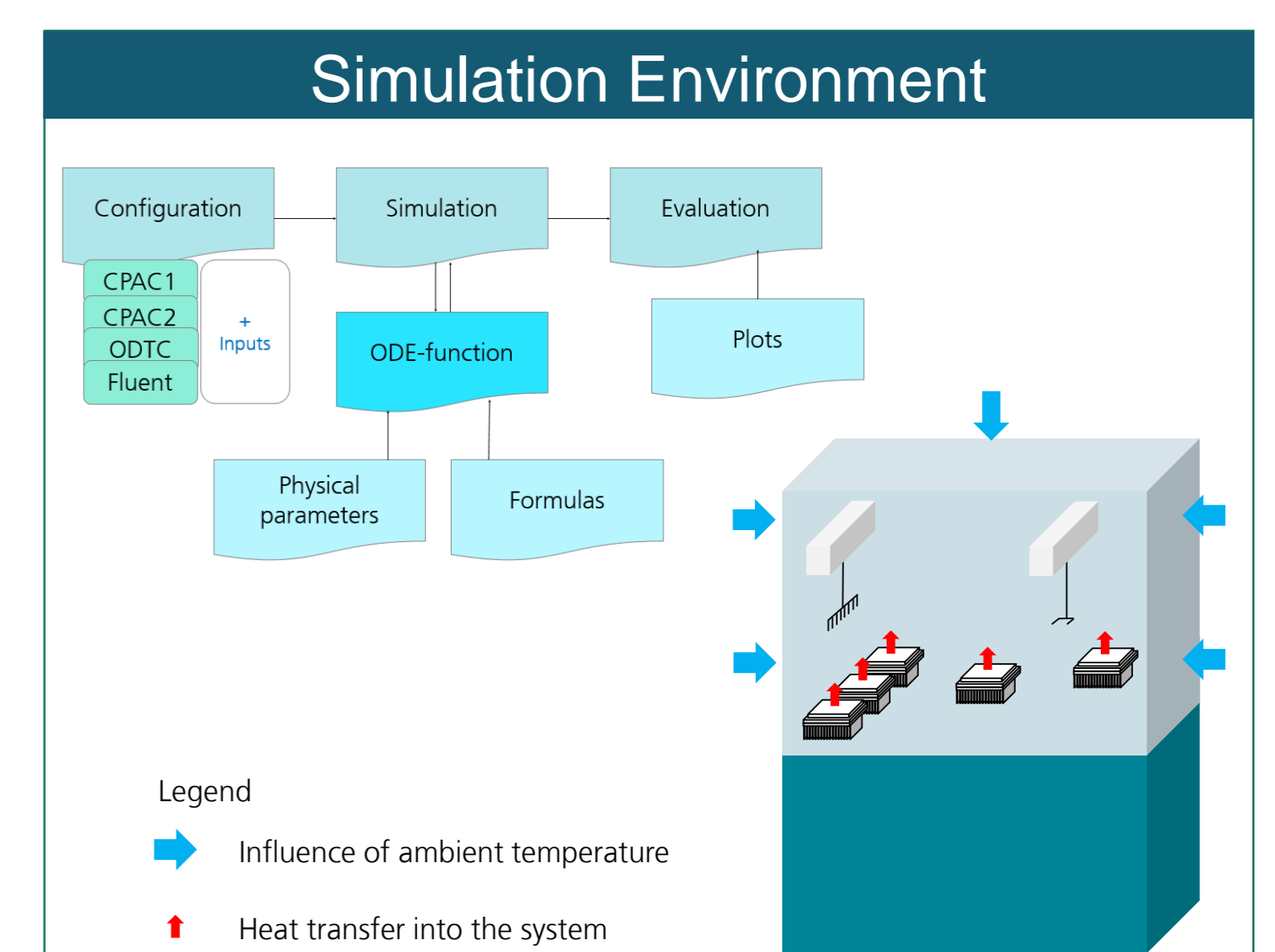


Figure 3: Schematic design of the liquid handling system with different devices.

## Results

- Mathematical models of various devices within the liquid handler such as thermocyclers, shakers and cooling systems, were created to understand their heat behavior
- Model design based on lumped-capacitance approach and equations approximating heat conduction and convection. An FDM approach was used to calculate the spatial heat distribution
- Configurable simulation environment, in which given device models can be added and positioned to represent an existing or planned liquid handling system
- Prediction of resulting temperature curves based on process target temperatures and other device states like e.g. opened lids
- Predictions of how the heat output of the devices and the overall system changes depending on different environmental conditions
- Prediction of the heat distribution in the liquid handling system over the entire process with a 3D visualisation

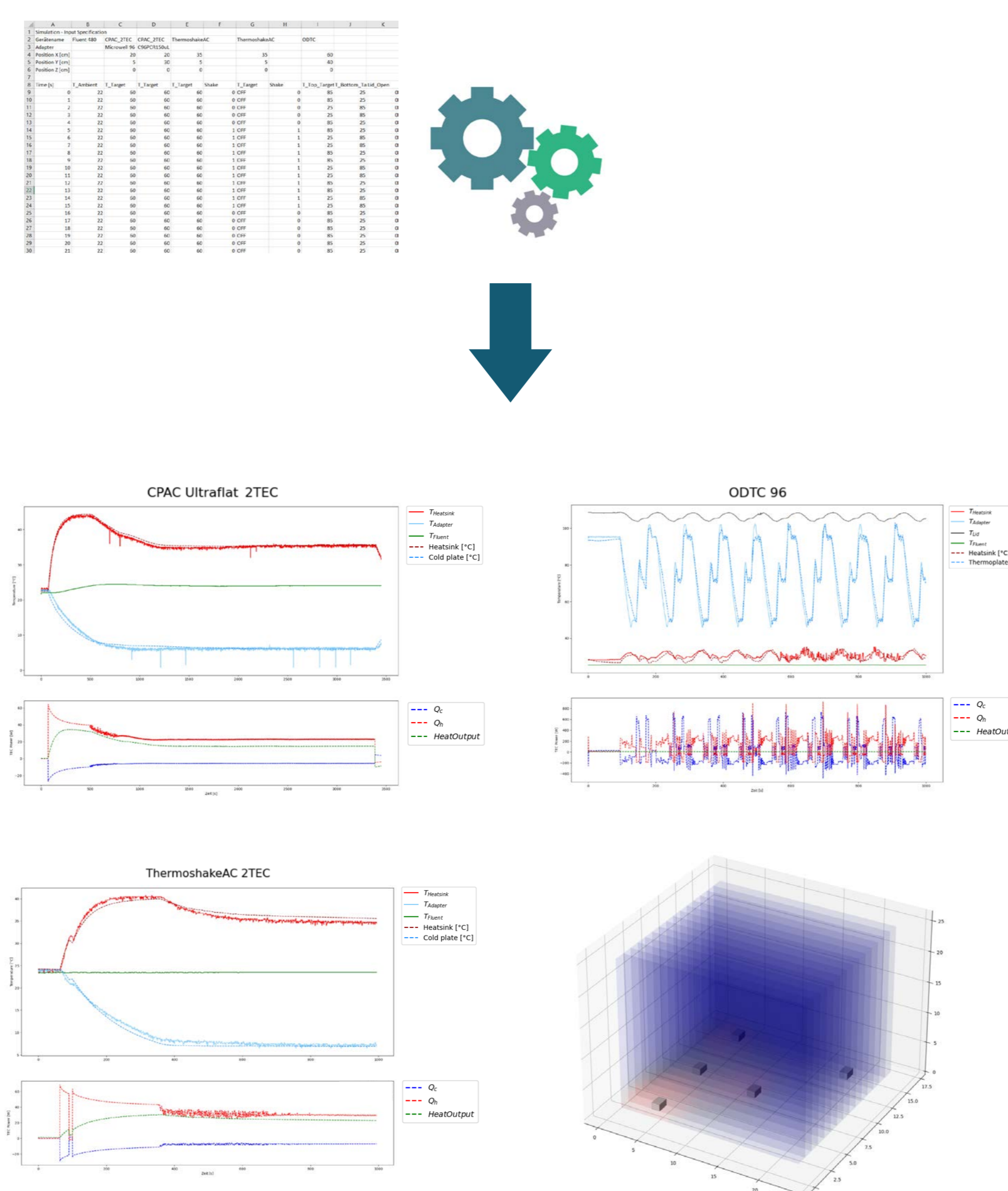


Figure 4: Simulation based on process table resulting in temperature curves for each device and the heat distribution in the liquid handling system as 3D visualisation

## Conclusion

The generated simulation environment allows to predict the temperature behavior in a liquid handling system. The system uses process parameters (duration of steps, target temperatures, device states etc.) as inputs to predict the behavior of each device and the overall system.

Since the simulation environment is freely configurable, the devices used, their number and their position in the liquid handling system can be adjusted. This means that different configurations can be tested quickly and easily and the optimal choice of the devices in the liquid handling system can be determined when designing or validating a process. In this way, valuable insights can be gained on how the system's design and operating parameters can be optimized to improve its thermal performance.