



Finite element modelling for the optimization of temperature control in Lab-on-a-Chip devices

T. Pardy^{a,b}, T. Rang^a, I. Tulp^b

^a Thomas Johann Seebeck Department of Electronics, Tallinn University of Technology, Tallinn, Estonia

^b SelfDiagnostics Deutschland GmbH, Leipzig, Germany

Abstract

Some of the assays actively developed in a Lab-on-a-Chip format require temperature control, mostly heating to a specified range for the duration of the assay. In a highly portable system with limited power supply, heating microliters of liquids poses technical challenges, which may be costly to overcome solely by experimental means.

The way computer-aided design helps in rapid prototyping, so does finite element modelling help in validating the functionality of these prototypes in silico, saving time and costs. The model we present was developed for the geometric optimization of Lab-on-a-Chip devices and tested for experimental setups emulating the targeted device format. The model is presented for multiple temperature control scenarios, i.e. heaters and device geometries.

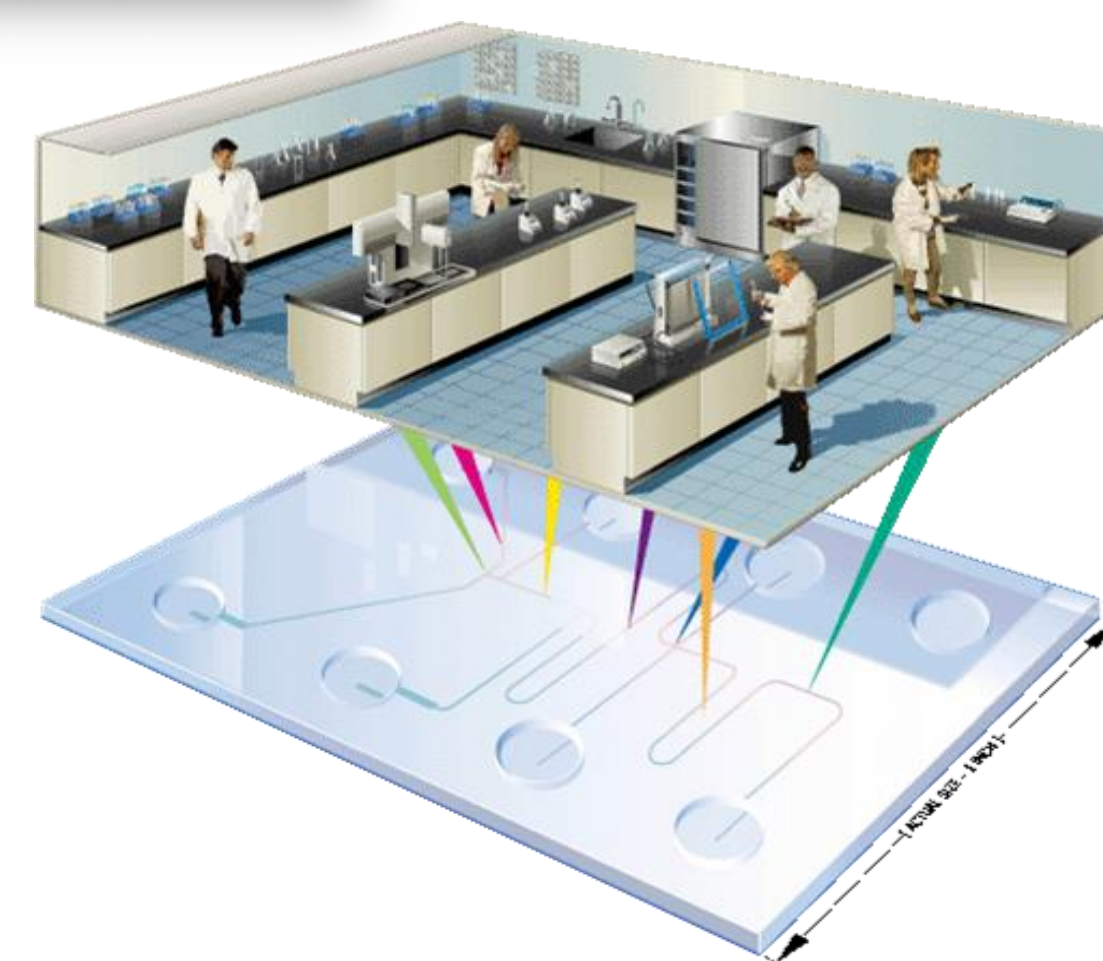


Fig. 1: The core concept of Lab-on-a-Chip devices is to fit the various functions required in a clinical assay workflow (i.e. liquid handling, heating etc.) into a tiny, portable device that is possible to use at the point of care. [3]



Fig. 2: An experimental setup with a heater prototype containing a mock-up of a microfluidic cartridge (75 mm x 25 mm). The NC milled PMMA structure contains a self-regulating resistive heating element and a temperature sensor for temperature recording.

Introduction

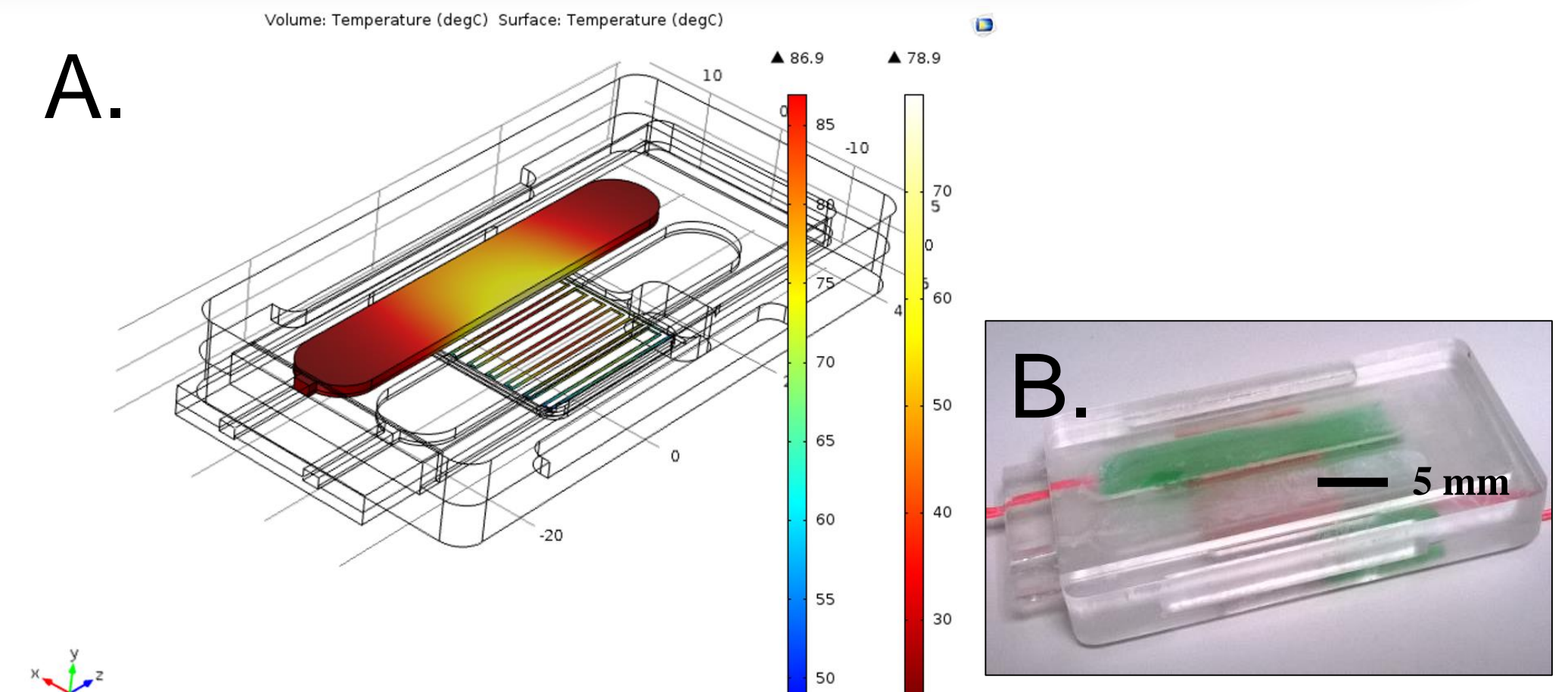


Fig. 3: Representation of an experimental setup in our finite element model: A milled plastic experimental setup (B.) with a resistive heater is modelled and the resultant heat map shown (A.). The model indicates that heat distribution in the microfluidic channel is highly non-uniform in this setup, and geometry must be optimized.

Finite element modelling is a well-established method for simulating dynamic systems either as stationary or time-dependent processes. Models fine-tuned with experimental data may help estimate temperatures at spatial points where sensors are impossible to fit. Additionally, these models can help assess the feasibility of a prototype structure in silico without the time and cost requirements of prototyping [2].

Active regulation

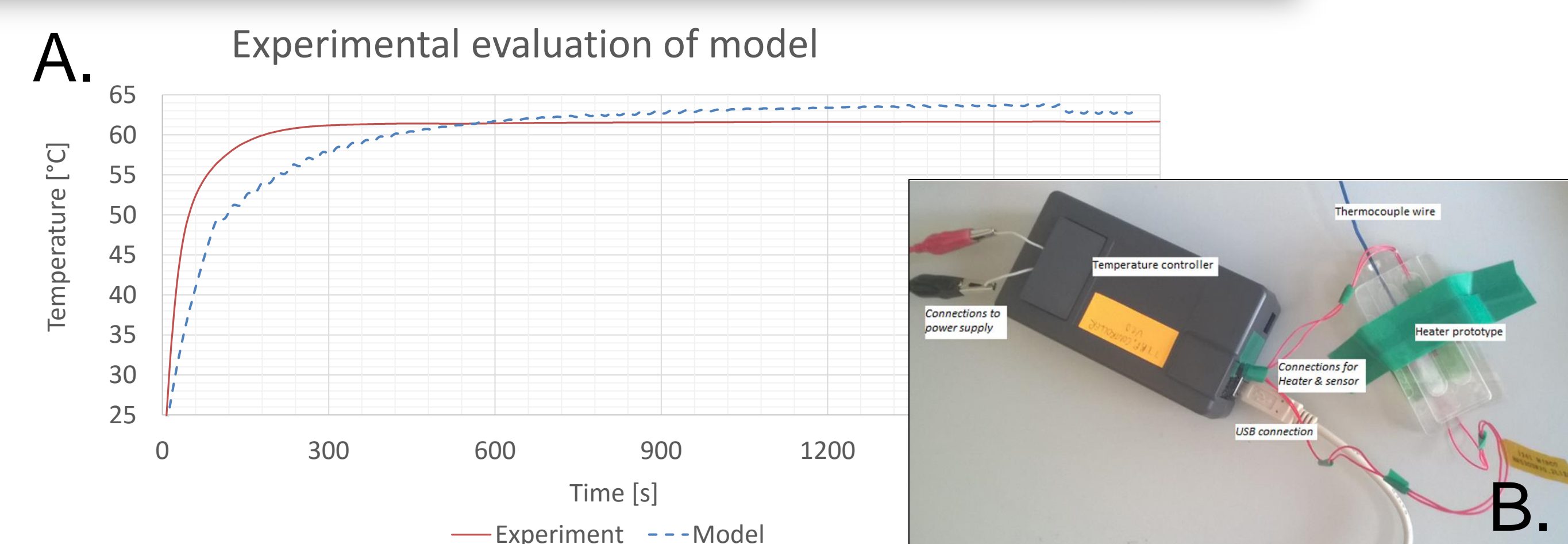


Fig. 4: An iteration of the model for actively controlled resistive heating elements. The mini thermostat (black enclosure in figure B.) was connected to the resistive heater in the setup shown in Fig. 3 (B.). Comparison of model results to experiments indicated a noticeable difference in predicted and real rise times (A.), due to the hysteresis of the physical thermostat that was not simulated in silico. The mean absolute error of the prediction was 2.3 °C.

A user-friendly, microcontroller-based mini thermostat was developed based on the Arduino Uno platform to support Lab-on-a-Chip molecular diagnostics devices that require temperature control. The expression for proportional control the thermostat used was plugged into our finite element model, and simulations done with experimental parameters. The model predicted experimental results with a mean absolute error of 2.3 °C, which decreases to 1.5 °C once the set point is reached.

Conclusion & outlook

The presented finite element model aims to help in the development of Lab-on-a-Chip devices which require temperature control. The model simulates the thermal system in such devices to enable in silico validation of designs and geometry optimization, and aims to be a versatile tool supporting multiple temperature control methods. At the current stage, the model could predict experimental results with an accuracy of 2.3 °C for actively regulated, and 1 °C for passively regulated heaters in the tested experimental setups.

References

- [1] <http://www.gene-quantification.de/lab-on-chip.html>
- [2] Pardy, T., T. Rang, and I. Tulp. "Finite element modelling of the resistive heating of disposable molecular diagnostics devices." *Computational Methods and Experimental Measurements XVII* 59 (2015): 381.
- [3] Pardy, T., T. Rang, and I. Tulp. "Modelling and experimental characterisation of self-regulating resistive heating elements for disposable medical diagnostics devices." *Materials Characterisation VII* 90 (2015): 263.

Passive regulation

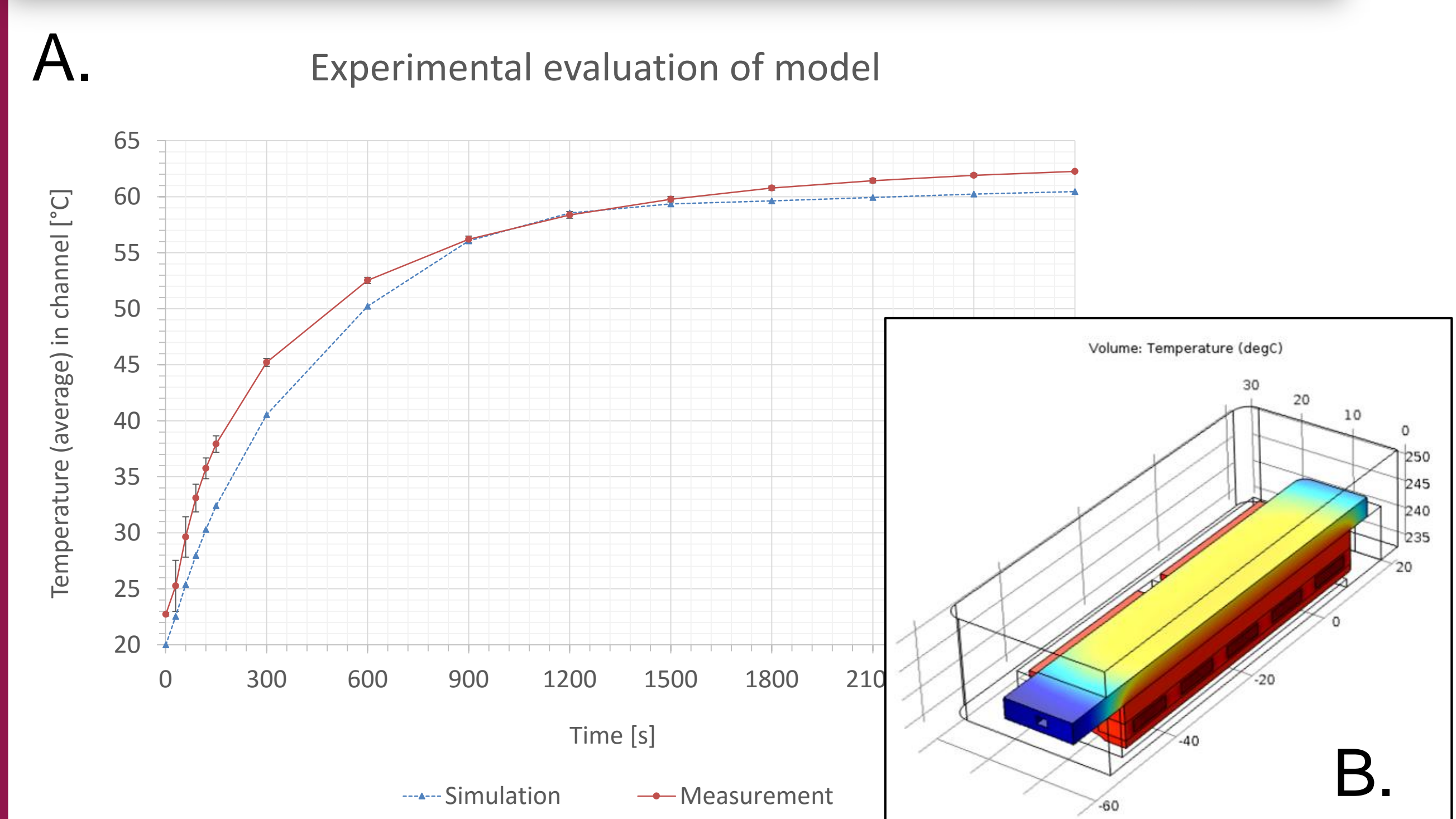


Fig. 5: An iteration of the model for self-regulating resistive heating elements. Heat maps show heater and channel interaction (B.) and can point out design errors and aid in optimizing temperature distribution inside the reaction chamber. At the current stage it is possible to estimate heat output with a mean absolute error of 1°C (A.).

An iteration of the microheater model was fine-tuned for self-regulating heaters [3], and evaluated with ceramic PTC (positive temperature coefficient) thermistors in a test structure milled from PMMA (shown in Fig. 2). The positive temperature coefficient of resistance effect is responsible for passive regulation: the resistance of a PTC heater rises exponentially beyond a defined temperature, thereby regulating current input and heat output. This set point is defined by doping and together with geometry optimization can yield regulation better than 1°C around the set point. For the experimental validation of the model, a commercially available PTC resistive heating element was used (DBK HP04-1/04-24).

Acknowledgments

The authors wish to thank for the support of the Sächsische AufbauBank provided under project SAB#100204668, and the Estonian Research Council provided under research projects SF0140061s12, ETF8592 and IUT19-11, and the Foundation Archimedes through the Centre of Excellence CEBE (TK05U01) for supporting technology-oriented scientific projects in Estonia. Additionally, the authors would like to express their gratitude to Jüri Oleitšuk for the manufacturing of test structures.