COMSOL MULTIPHYSICS® SIMULATION OF ENERGY CONVERSION AND STORAGE CONCEPTS BASED ON OXIDE CRYSTALS

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Background

Introduction

A mathematical model based on a finite element method (FEM) is presented as an initial approach for a system converting waste heat energy into chemical energy. This system consists of a pyroelectric $LiNbO_3$ plate placed into a cylinder which undergoes a laminar water flow with an appropriate periodic heat source. It solves the heat transfer equation in non-isothermal flow, where the density of process fluid varies in the presence of an inhomogeneous temperature field $T(r,t)$ in space r and time t. In addition, a pyroelectric current and the resulting polarization are calculated. The harvested energy can be used for pyrocatalytic water splitting, which in turn can be utilized for electricity generation from fuel cells.

Pyroelectricity

- Heating cycle starts (i) by increasing the temperature to value T_H.
- Polarization decreases. Charge/current generation (ii).
- Cooling cycle starts (iii) by decreasing the temperature to value T_K.
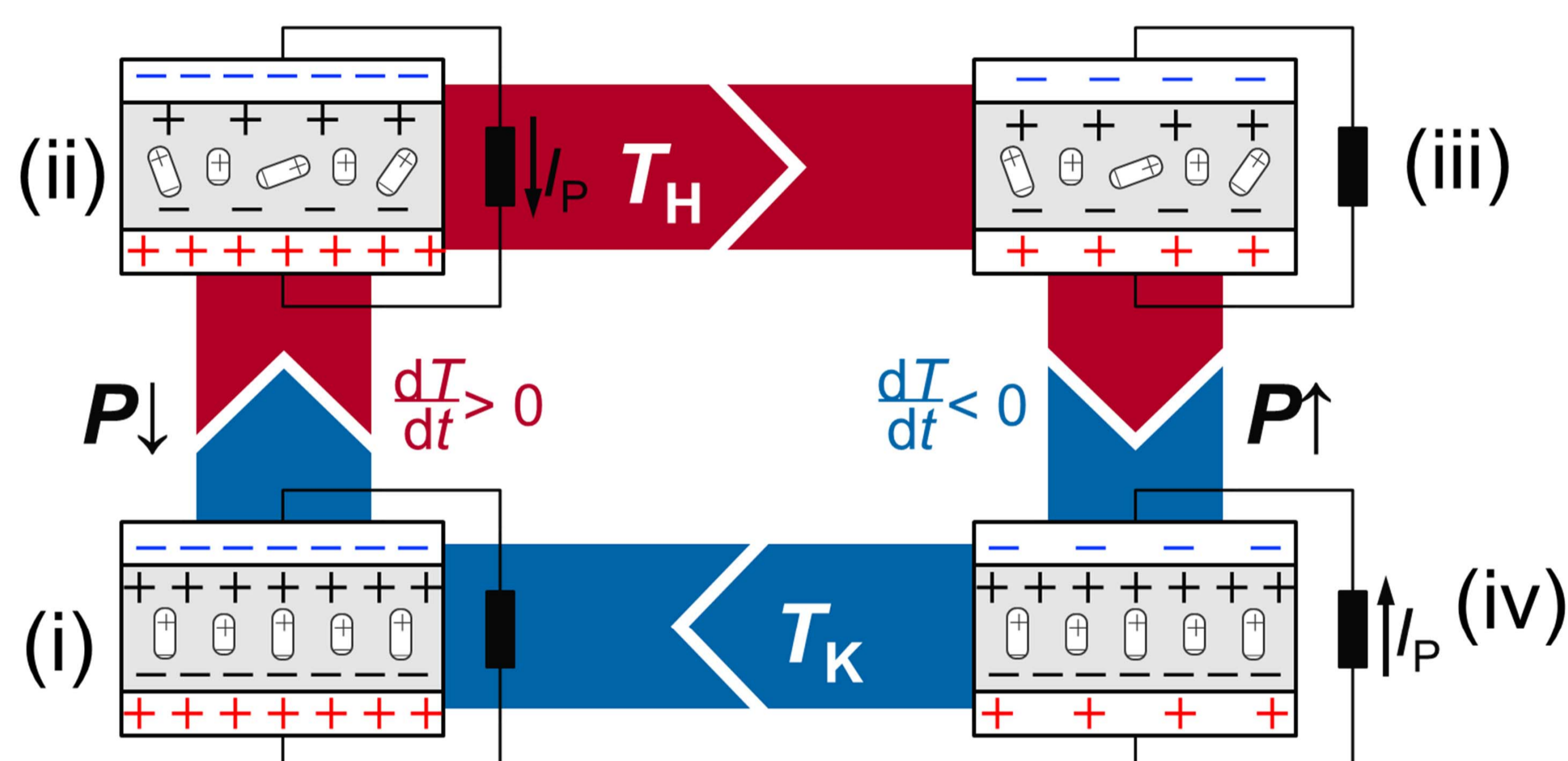- Polarization of the crystal increases. Current generation (iv).

Figure 1: Surface charge generation due to the change of the spontaneous polarization during heating and cooling cycle of the pyroelectric material (© by Clemens Forman).

Computational Methods

FEM was utilized using the COMSOL Multiphysics® code. The conjugate heat transfer interface contains the fully compressible formation of the continuity equation (1) and momentum equation (2) as well as the heat transfer in solid equation (3):

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \boldsymbol{u}) = 0 \quad (1)$$

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \boldsymbol{F} \quad (2)$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\boldsymbol{u} \cdot \nabla) T \right) = -(\nabla \cdot q) - \boldsymbol{Q} \quad (3)$$

Where ρ is the density, u is the velocity, p is the pressure, F is the body force vector, C_p is the specific heat capacity, q is the heat flux by conduction and Q is the viscous heating of the periodic heat source (frequency of 50 mHz, $T_{min} = 300$ K, $T_{max} = 380$ K and ambient temperature $T_{amb} = 340$ K). Material properties of $LiNbO_3$ are used for all simulations.
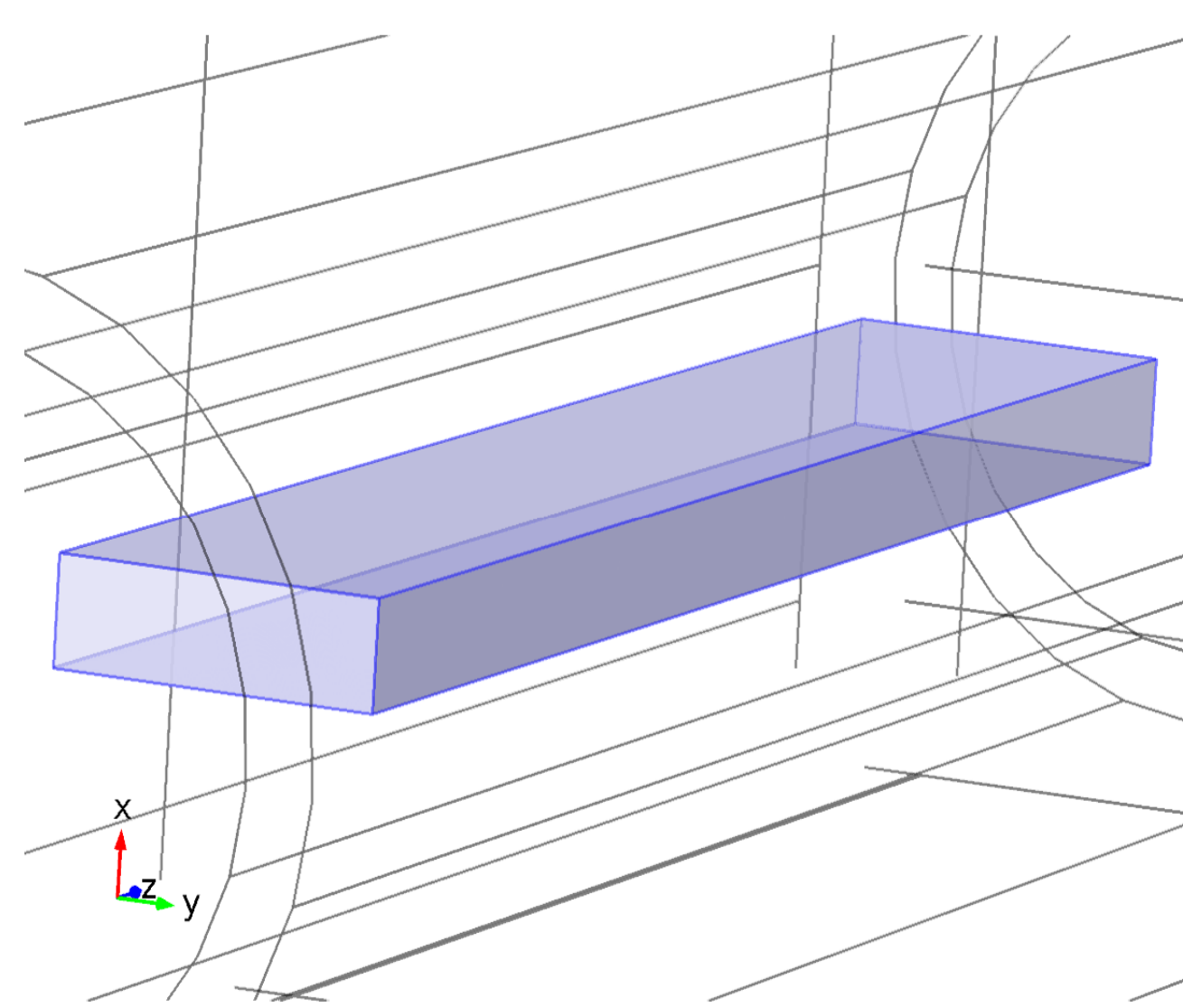

Figure 2: 3D-model of the $LiNbO_3$ ($d = 2$ mm) as pyromaterial plate placed into a cylinder undergoing a laminar water flow

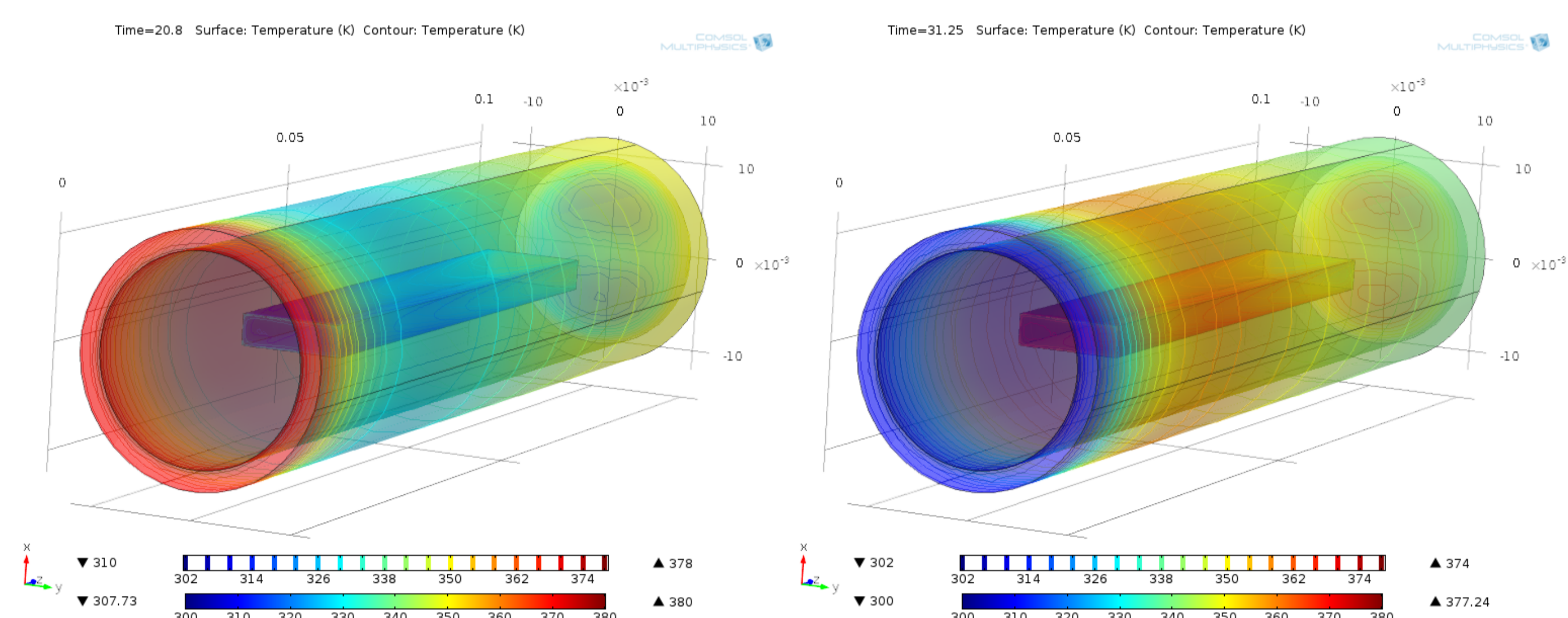# Results

Heat transfer equation

Figure 3: 3D-model of the temperature distribution $T(r,t)$ after the cooling cycle (left) and the heating cycle (right). The periodic heat source is placed in the direction of the flow (front of the image).
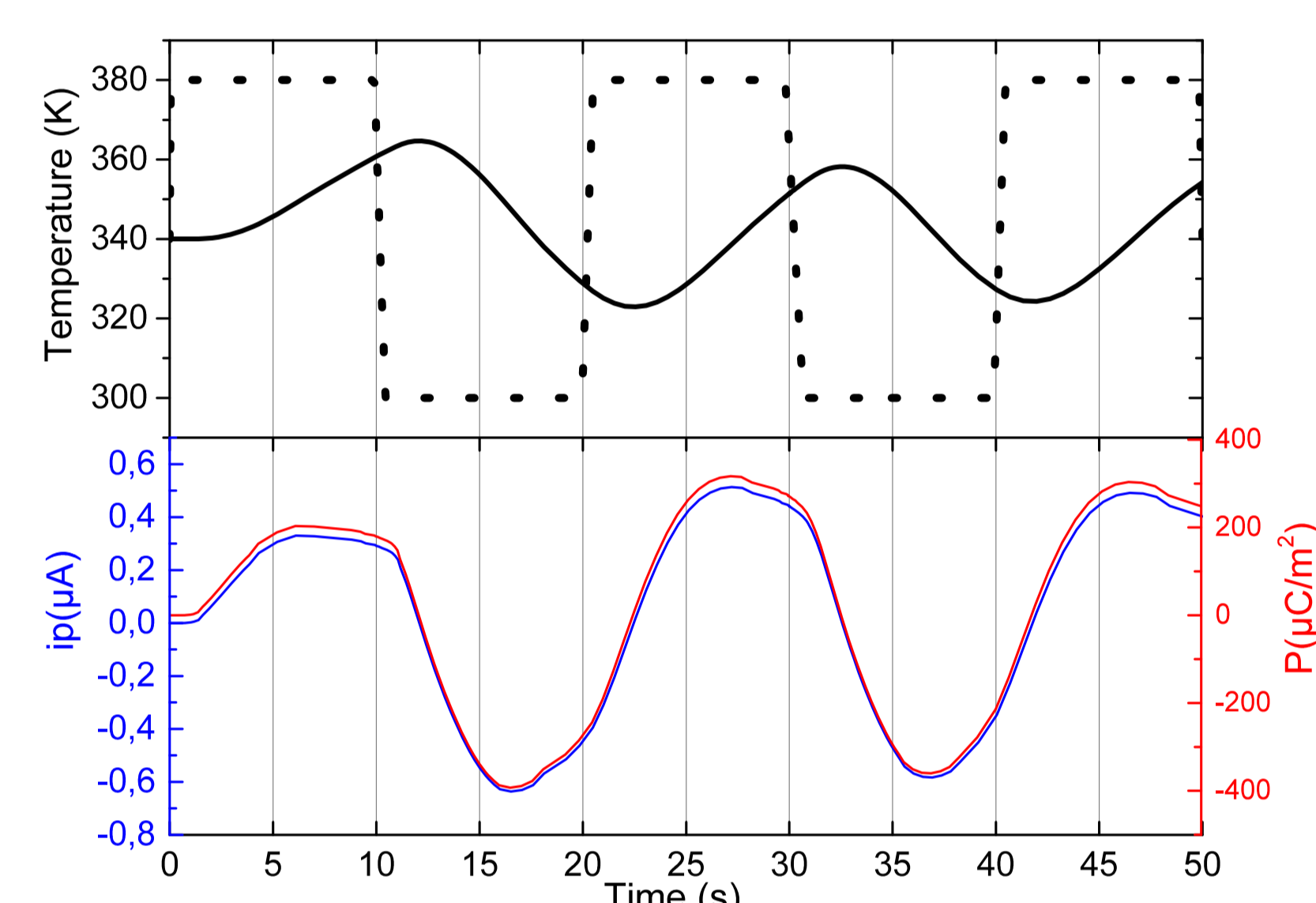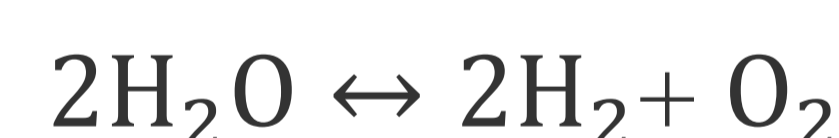

Figure 4: Temperature over time of pyroelectric plate compared to the temperature profile of the heat source (dotted line), calculated pyroelectric current Ip (blue) and polarization P (red)

Application: Water splitting/fuel cell

$$2H_2O \leftrightarrow 2H_2 + O_2$$

➤ For $U = 10^3$ V:

$$N_{H_2} = \frac{A \, \Delta P}{2e_0} = \frac{Q}{2e_0} = 7 \cdot 10^{11} \ (\approx 10^{-9} \text{ mol} \ \approx 10^{-7} \text{l}) \text{ per cycle}$$
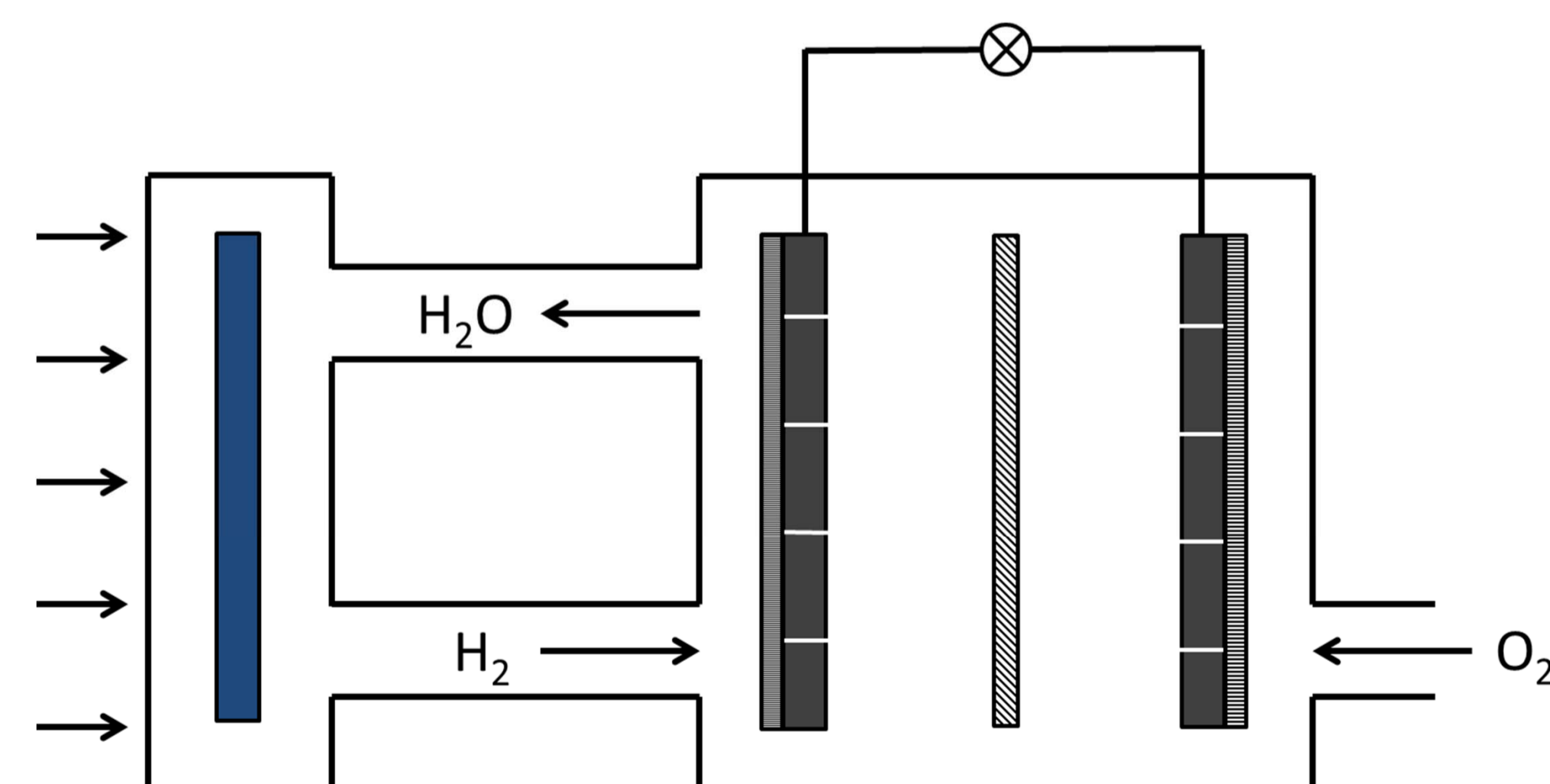

Figure 5: Pending patent for the combination of a fuel cell and a pyroelectric material as a concept for a new energy storage device.

Conclusion

A system converting heat energy into chemical energy is modelled by COMSOL Multiphysics®. It solved the heat transfer equation in solid undergoing a laminar water flow using a periodic heat source. The temperature distribution equation T(r, t) was used to estimate the pyroelectric current and the polarization of the pyromaterial. This simple model can be used for modeling of electric field and the potential difference between the top and the bottom of the pyromaterial plate. The produced voltage can be applied for pyrocatalytic water splitting for H_2 production from fuel cells, for instance.

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