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A simple tool for the modeling of heat flow calorimeters

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Abstract

A simple and inexpensive tool for the modeling of heat flow calorimeters is presented. The tool is based on the RC analogy. The easy use has to be payed by restrictions concerning the symmetry of the calorimetric configuration which has to be modeled. Despite of the simplicity of the model results of practical relevance can be obtained.

Keywords: Heat conduction calorimeter; IC calorimeter; RC model; Simulation

1. Introduction

There are at least two reasons for modeling of heat transfer in calorimeters. The first one is the need for a model in order to calculate the generated heat power by deconvolution of the measured calorimetric signal. Further, the modeling of the heat transfer is useful if systematic errors caused by sensitivity gradients have to be estimated. The latter is of special importance in miniaturized heat flow calorimeters because of the incomplete heat power integration in such systems [1,2]. For example, in a micro-sized reaction chamber of a chip calorimeter the sensitivity change can take values up to 50% dependent on the local position of the heat power dissipation source. In addition, it is mostly difficult to find suitable calibration reactions for micro-sized calorimeters. Therefore, the modeling of the temperature distribution within a calorimeter dependent on the position of the heat source could be helpful.

Modeling of the heat transfer in any configuration is more or less a basic task. For this, a lot of powerful tools are available. Software packages like ANSYS [3] apply finite element methods. In general, they are very complex and not comfortable for the simulation of dynamic processes. Further some experience is necessary to obtain stable solutions. A much more easy way is to apply the RC analogy for the construction of suitable models. From a physical point of view, it provides comprehensible results and its implementation as well as its application using standard mathematical software is easy. For didactic purposes, we have developed a simple software tool for signal simulation in heat flow calorimeters based on RC analogy. The programs are written in MATLAB, a wide-spread used mathematical software system [4] which is nowadays learned by students in the first courses. As it will be shown, the developed tool can be applied successfully also to more complex configurations despite of their simplicity.

2. RC-models

The application of the RC analogy for modeling of the heat transfer in calorimeters is not new [5]. Therefore, only a brief summary of the basic concept will be given. The basic RC analogy considers the device as network of N heat capacities C_i. Two localized heat capacities C_i and C_j are coupled by the thermal resistance R_{ij} (Fig. 1). Every C_i can also be connected to the surroundings by R_{i0}. In Fig. 1, the simple case of a uniform external temperature T_0 is assumed. The state of the system is determined by the set of the temperatures T_i of every network-node. Selected temperatures T_i (e.g. $j1$, $j2$, the cold junction and hot junction temperature of a thermocouple) provide the calorimetric signal $u(t)$. Heat power dissipation $W_i(t)$ can be generated in any network-node. Eqs. (1)–(4) give a mathematical description of the system. In Eq. (2), the external temperature T_0 serves

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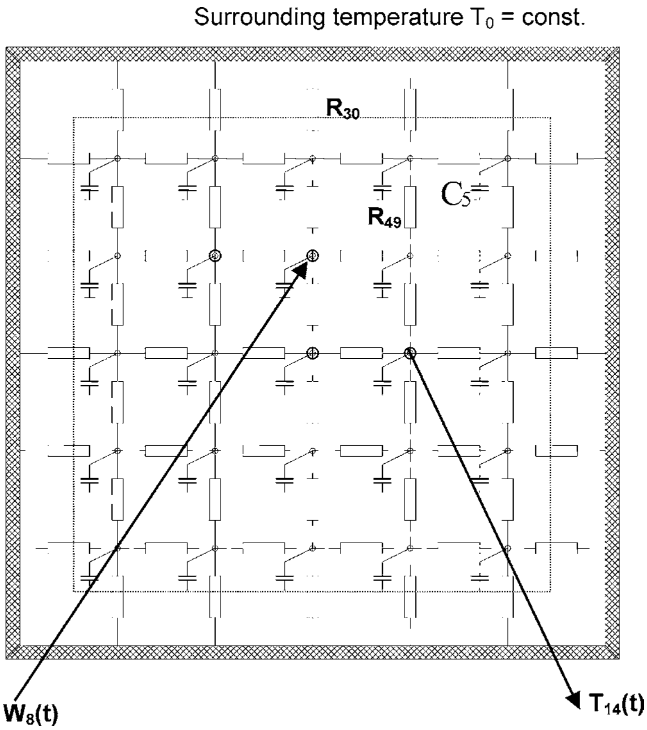

Fig. 1. RC network as a model for a heat flow calorimeter (W_8: heat power dissipation in element 8; T_{14}: temperature of element 14; C_5: heat capacity of element 5; R_{49}: thermal resistance between elements 4 and 9; R_{30}: thermal resistance between element 3 and thermostat).

as reference. For simplification the coupling resistances to the surroundings R_{i0} are written as R_{ii}. The matrix Eqs. (3) and (4) represent the standard form of a state-space description of a linear system. In this form a direct implementation in MATLAB syntax is possible.

$$W_i(t) = C_i \frac{dT_i}{dt} + \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{1}{R_{ij}}(T_i - T_j) + \frac{1}{R_{i0}}(T_i - T_0) \quad (1)$$

with $R_{ii} = R_{i0}$, $T_0 = T_{\text{ref}}$,

$$\frac{dT_i}{dt} = -\frac{1}{C_i}\sum_{j=1}^{N}\frac{1}{R_{ij}}T_i + \frac{1}{C_i}\sum_{\substack{j=1 \\ j \neq i}}^{N}\frac{1}{R_{ij}}T_j + \frac{1}{C_i}W_i \quad (2)$$

$$\underline{\frac{dT}{dt}} = \underline{A}\,\underline{T} + \underline{B}\,\underline{W} \quad (3)$$

with $a_{ii} = -\frac{1}{C_i}\sum_{j=1}^{N}\frac{1}{R_{ij}}T_i$,

$$a_{ij} = \frac{1}{C_i}\frac{1}{R_{ij}}T_j, \qquad b_i = \frac{1}{C_i}$$

$$u(t) = \underline{C}\,\underline{T} + \underline{D}\,\underline{W} \quad (4)$$

with $c_{j1} = -k_{\text{seeb}}$, $c_{j2} = k_{\text{seeb}}$, $\underline{D} = 0$,

where k_{seeb} is the Seebeck coefficient.

3. MATLAB modeling tool

The developed MATLAB tool consists of three programs (LAYER, ADDLAYER and MKMODEL). Aim of the tool is the calculation of the matrices $\underline{A}$, $\underline{B}$ and $\underline{C}$ (Eqs. (3) and (4)) on the basis of the design of the configuration of the calorimeter. The matrices can be applied for the signal simulation using the available standard MATLAB procedures (see Appendix A). Precondition of the application of the tool is a cylindrical symmetry of the configuration, i.e. an appropriate approximation has to be performed. As for example outlined in Fig. 2, the configuration is assumed as a composition of cylindrical layers, everyone consisting of several concentric ring elements. By use of the programs, the following tasks can be executed:

LAYER: A data structure describing the layer as a subsystem is generated. Necessary input information are the radii of the ring elements of the layer, the thickness of the layer and some parameters of every ring element (density, specific heat capacity, thermal conductivity, coupling indices).

ADDLAYER: It connects the layers described by the data structure produced above to a complete system. The output data structure contains the system matrices of the composed system.

MKMODEL: The program completes the system by connecting the surface elements to the surroundings via the specified coupling resistances. Further it defines the input and output signals, respectively. Output of the program is the set of system matrices applicable for signal simulation.

How the programs have to be used is explained in detail in the Appendix A. The programs are provided on request by the authors.

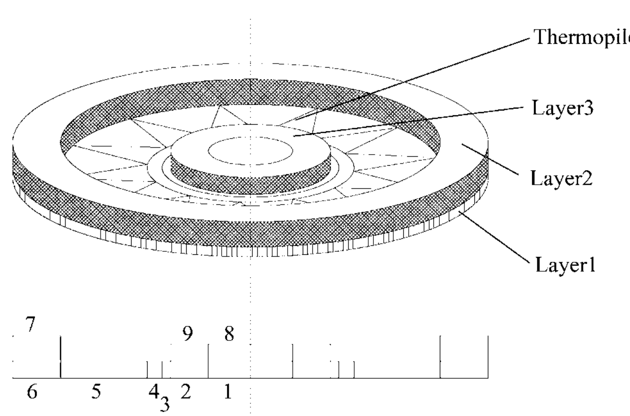

Fig. 2. Model structure of a chip calorimeter coated with a polymer film (element 1–6: silicon membrane; element 7: silicon rim; element 8–9: polymer film).

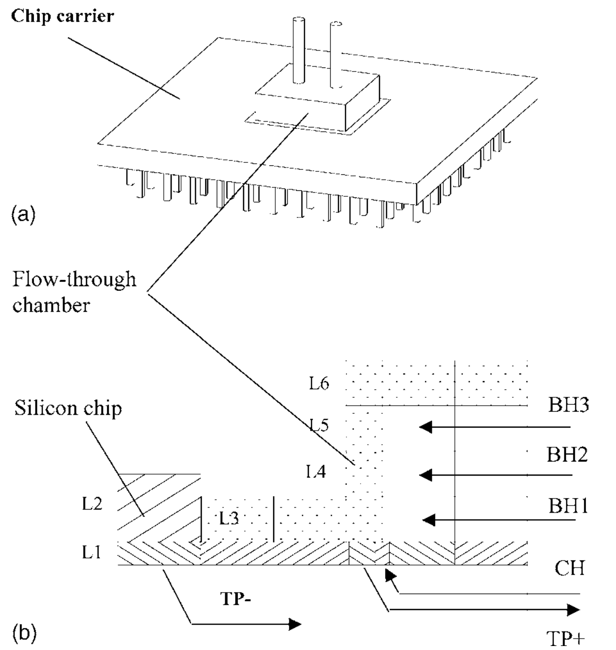

Fig. 3. Model structure of a flow-through calorimeter with 6 layers and 21 elements. (a) Sketch of the calorimeter, (b) model structure (BHi: bulk heater positions; CH: chip heater position; TP+, TP: the position of the hot and cold junctions of the thermopile).

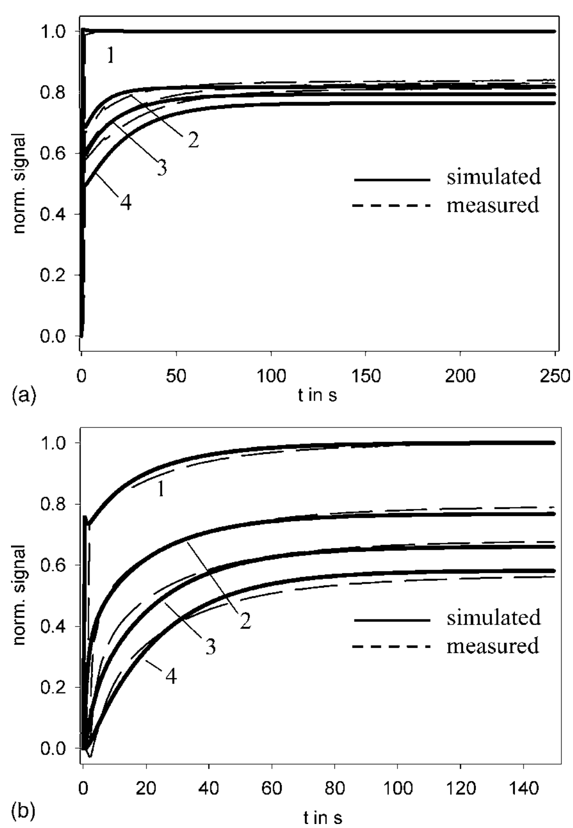

Fig. 4. Comparison of measured and simulated step response signals. (a) Chip heater response (1: chip without chamber; 2: empty chamber; 3: chamber filled with ethanol; 4: chamber filled with water), (b) chip and bulk heater response, chamber filled with ethanol (1: chip heater; 2: bulk heater position 1; 3: bulk heater position 2; 4: bulk heater position 3).

4. Example of application

As mentioned above, the analysis of sensitivity changes in micro-sized calorimeters is of practical importance. In order to examine the vertical sensitivity changes in the reaction chamber of a micro-sized flow-through calorimeter, Joule heating experiments were performed using heaters at different local positions (for experimental details see [2]). Step response signals were analyzed and modeled by the described software tool. The goal of the simulation was to get an idea of the influence of the chamber size, the choice of the material of the chamber as wells as the thermal parameters of the applied fluids. To be able to apply the simulation tool the square symmetry of some parts of the configuration has to be converted to cylindrical one ($r_i = 1/\sqrt{a_i}$, r_i is the radius of the element i, a_i the side length of the element i). Fig. 3 depicts the structure of the applied model. In Fig. 4, measured response curves are compared with simulated signals. The signals are normalized by the steady-state values of the signals of the free chip. The simulated curves are not a result of a fit. They are calculated on the basis of the known geometric and physical parameters. Only the heat exchange coefficient for the heat transfer with the surroundings was tuned manually. It is obvious that despite of the simplicity of the model the accordance of experimental and simulated signals is quite well. Of course, more sophisticated models which are considering the real symmetry of the calorimeter in a greater extend will give improved results [5].

5. Conclusions

The RC analogy provides simple and comprehensible models of heat flow calorimeters. If some restrictions concerning the symmetry of the configuration are acceptable derived tools for signal simulation are inexpensive and easy to use. The simulation results are sufficient enough for qualitative studies and for didactic use.

Acknowledgements

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Appendix A

The following MATLAB program is an example for the use of the developed modeling tool. In the first part, the model is defined by the parameters of the layers. After that the model matrices will be calculated by use of the programs of the modeling tool. At the end, a step response signal is simulated.

```
% Model_1
%
%
global  param  Pg  Si  Wa  Et  cs  la  ro  dm  alph  sk         % constants
% Parameter of the materials (Pg- polymer, Si – silicon, Wa – water, Et – ethanol)
%           Pg        Si      Wa       Et
param = [1448     705    4180     2340; ...     % cs in J kg-1 K-1    (specific heat capacity)
            0.26      148   0.608   0.180; ...     % la in W m-1 K-1   (thermal conductivity)
           1410     2330   1000      789  ] ;       % rho in kg m-3      (density)
%
Pg = 4; Si = 5; Wa = 6; Et = 7;
cs = 1; la = 2; ro = 3;
%
alph = 32;                   % heat transfer to air  inW m-2 K-1
ralphiso = 400;           % heat transfer through glue
sk = 0.050;                % seebeck coeff in V K-1
dm = 25e-6;                % thickness of Si membrane in m
df = 0.5e-3;                % thickness of the silicon rim
ds = 5e-6;                   % thickness of the polymer film

% Definition of the Layers:
% Layer1:  silicon membrane,  containing elements 1 to 6
ra11 = [0    1.6  1.9  2.1    2.46  4.51]*1e-3;        % inner radii  of the elements
ra12 = [1.6 1.9  2.1  2.46  4.51  5.65]*1e-3;        % outer radii   of the elements
ra1 = [ra11' ra12'];
d1 = dm*ones(1,6);                                          %  thickness of the layer
ma1 = [Si Si Si Si Si Si];                                %  material of the elements
dlink1 = {zeros(1,6)};                                     %  no connection to other elements
ralph1 = ralphiso;                                           %  radial thermal coupling to surroundings
saxtl1 = [0 0 1 1 1 0;0 0 alph alph alph 0]';          % axial to top coupling to surroundings
saxbl1 = [1 1 1 1 1 1; alph alph alph alph alph alph]';    % axial to bottom couplin g
%
% Layer 2: silicon rim, one ring
ra2 = [4.51 5.65]*1e-3;
d2 = df;
ma2 = Si;
dlink2 = {6};                                                    % coupling to element 6
ralph2 = ralphiso;
saxtl2 = [1 alph];


saxbl2 = [0 0];
%
% Layer3:  polymer film, element 8 and 9
ra31 = [0 1.6]*1e-3;
ra32 = [1.6 1.9]*1e-3;
ra3 = [ra31' ra32'];
d3 = [ds3 ds3];
ma3 = [Pg Pg];
dlink3 = {1 2};                                                 % coupling to element 1, 2
ralph3 = alph;
saxtl3 = [1 1; alph alph]';
saxbl3 = [0 0; 0 0];
%

% Definition of the input and output elements
OutpM = 6;                      % cold junctions
OutpP =  4;                     % hot junctions
Inp = 3;                          % Joule heating (position of the integrated heater)

% Assembly of the model
L1 = LayerB(d1, ra1, ma1, dlink1, ralph1, saxtl1, saxbl1);
L2 = LayerB(d2, ra2, ma2, dlink2, ralph2, saxtl2, saxbl2);
L3 = LayerB(d3, ra3, ma3, dlink3, ralph3, saxtl3, saxbl3);
M1 = AddLayerB(0,L1);
M2 = AddLayerB(M1,L2);
M3 = AddLayerB(M2,L3);
[A, B, C, D] = MkModelB(M3, Inp, OutpM, OutpP);
%
%
% simulation of the step response
T = [0:0.1:250];                         % time scale
W = ones(size(T));                       % power step 1 W
Sys = ss(A,B,C,D);
u = lsim(sys,W,T);                        % simulation of the step response
plot(T,u), xlabel('t (s)'), ylabel('U (V)')
```

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