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Numerical simulations for nano-flow generator of VSL

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1 Introduction

The aim of this text is to formulate a physical model of processes which occur in the nano-flow generator of VSL which is based on a thermal expansion of water enclosed in a titanium reservoir, to identify the components of the flowrate which cannot be calculated analytically and to compute these components numerically using a COMSOL software.

2 Physical model of the nano-flow generator

If m(t) is a mass contained in the system in front of the meter under test (heated reservoir, cooling pipe, connecting parts) as a function of time and ρ_{out} is a density of water coming from the system in front of the MUT then the volumetric flow rate coming to the MUT is given by

$$Q = -\frac{1}{\rho_{out}} \frac{dm}{dt}.$$
(2.1)

The mass contained in the system is given as

$$m(t) = \int_{V(t)} \rho(x, t) dV$$
(2.2)

where V(t) is the interior space of the system (inside the reservoir and tubing) which can change with time due to thermal expansion of the reservoir and tubing and $\rho(x, t)$ is a density of water inside the system as a function of time and position. The time derivative of mass inside the system is then given as

$$\frac{dm}{dt} = \int_{V(t)} \frac{\partial \rho(x,t)}{\partial t} dV + \int_{\partial V(t)} \rho(x,t) \vec{\xi}(x,t) d\vec{S}$$
(2.3)

where $\partial V(t)$ is a boudary surface of the system and $\vec{\xi}(x,t)$ is a velocity of points at the boundary of the system. For example in the titanium reservoir $\partial V(t)$ is the boundary surface between water and titanium and $\vec{\xi}(x,t)$ is velocity of points at this boundary which are moving due to the thermal expansion of the titanium reservoir.

The complete system consists of a part which is heated in thermal bath and a part where the water is cooled to the ambient temperature again. We can split the space of the system V(t) and its boundary $\partial V(t)$ into two parts corresponding to the heated (index H) and cooled (index C) part. Then we get

$$\frac{dm}{dt} = \int_{V_H(t)} \frac{\partial \rho(x,t)}{\partial t} dV + \int_{\partial V_H(t)} \rho(x,t) \vec{\xi}(x,t) d\vec{S} + \int_{V_C(t)} \frac{\partial \rho(x,t)}{\partial t} dV + \int_{\partial V_C(t)} \rho(x,t) \vec{\xi}(x,t) d\vec{S}.$$
(2.4)

The first term is discussed in Section 3 and the second term is discussed in Section 4. The third and fourth terms are small and they are discussed in Section 5. In fact, in case the cooling down to ambient temperature is instantaneous, these terms are zero. These terms are also zero in case T(x, t) over the capillary is not a function of time.

3 Thermal expansion of water in the reservoir

Now we will focus on the first term of (2.4) in more detail. This term is the main term in flowrate calculation and describes the thermal expansion of water in the reservoir itself.

3.1 Physical model for the thermal expansion term

In the reservoir there is a thermometer inserted. We denote $T_M(t)$ the temperature as measured by this thermometer. This temperature is a function of time. Consider the temperature field in the system T(x,t) in a form

$$T(x,t) = T_M(t) + \Delta T(x,t).$$
 (3.1.1)

The water density is a function of temperature and pressure. We neglect the density changes due to pressure change and we consider only the temperature dependence of the density. In this work the Tanaka formula for degassed water was used. According to this formula we have

$$\rho = a_5 \left(1 - \frac{(T+a_1)^2 (T+a_2)}{a_3 (T+a_4)} \right)$$
(3.1.2)

where *T* is temperature in °C and $a_1 = -3.983035$ °C, $a_2 = 301.797$ °C, $a_3 = 522528.9$ °C², $a_4 = 69.34881$ °C, $a_5 = 999.9714 kgm^{-3}$. The time derivative of the density is then given as

$$\frac{\partial \rho(T(x,t))}{\partial t} = \frac{\partial \rho}{\partial T} \frac{\partial T}{\partial t}.$$
(3.1.3)

By means of a Taylor expansion, the temperature derivative of density can be written as

$$\frac{\partial\rho(T)}{\partial T} = \frac{\partial\rho(T_M(t) + \Delta T(x,t))}{\partial T} \approx \frac{\partial\rho(T_M(t))}{\partial T} + \frac{\partial^2\rho(T_M(t))}{\partial T^2} \cdot \Delta T(x,t)$$
(3.1.4)

where the second and higher order terms are neglected. Combining equations (3.1.3) and (3.1.4) we have

$$\frac{\partial \rho}{\partial t} = \left(\frac{\partial \rho \left(T_M(t)\right)}{\partial T} + \frac{\partial^2 \rho \left(T_M(t)\right)}{\partial T^2} \cdot \Delta T(x,t)\right) \left(\frac{dT_M(t)}{dt} + \frac{\partial \Delta T(x,t)}{\partial t}\right).$$
(3.1.5)

Dropping the second order term we obtain

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho \left(T_M(t) \right)}{\partial T} \cdot \frac{dT_M(t)}{dt} + \\
+ \frac{\partial^2 \rho \left(T_M(t) \right)}{\partial T^2} \cdot \frac{dT_M(t)}{dt} \cdot \Delta T(x, t) + \\
+ \frac{\partial \rho \left(T_M(t) \right)}{\partial T} \cdot \frac{\partial \Delta T(x, t)}{\partial t}.$$
(3.1.6)

Therefore for the first term in (2.4) we obtain

$$\int_{V_{H}(t)} \frac{\partial \rho(x,t)}{\partial t} dV = \frac{\partial \rho(T_{M}(t))}{\partial T} \frac{dT_{M}(t)}{dt} \cdot V_{H}(t) + \frac{\partial^{2} \rho(T_{M}(t))}{\partial T^{2}} \cdot \frac{dT_{M}(t)}{dt} \int_{V_{H}(t)} \Delta T(x,t) dV + \frac{\partial \rho(T_{M}(t))}{\partial T} \cdot \int_{V_{H}(t)} \frac{\partial \Delta T(x,t)}{\partial t} dV.$$
(3.1.7)

The first term of this formula is the main and the largest one. The second and third terms are correction terms. The second term represents a contribution of non-homogeneity of the thermal expansion coefficient $\partial \rho / \partial T$, i.e. $\partial \rho / \partial T$ is a function of position in space. The third term represents a contribution of non-homogeneity of temperature increase, i.e. $\partial T / \partial t$ is a function of position in space. In case of uniform temperature increase, this term will go to zero.

The second term reduces with reducing $\frac{\partial^2 \rho(T_M(t))}{\partial T^2}$. Relatively, this term reduces when the ratio of $\frac{\partial^2 \rho(T_M(t))}{\partial T^2}$ over $\frac{\partial \rho(T_M(t))}{\partial T}$ reduces. From equation (3.1.2) we have:

$$\frac{\partial \rho(T)}{\partial T} = \frac{a_5}{a_3} \left(\frac{(T+a_1)^2 (T+a_2)}{(T+a_4)^2} - \frac{(T+a_1)(3T+a_1+2a_2)}{T+a_4} \right)$$

and

$$\frac{\partial^2 \rho(T)}{\partial T^2} = \frac{a_5}{a_3} \left(-\frac{2(T+a_1)^2(T+a_2)}{(T+a_4)^3} + \frac{(T+a_1)(6T+2a_1+4a_2)}{(T+a_4)^2} - \frac{(6T+4a_1+2a_2)}{T+a_4} \right)$$

In the below figure the first and second order derivative of the density with respect to temperature are plotted. From this picture it follows that the second correction term reduces, absolutely and relatively compared to the first term, when the temperature increases.



In the formula (3.1.7) all quantities are known or measured besides the integrals of temperature and its time derivative. Estimations for these integrals are subject of numerical simulations and thus the goal of this report. The volume of the heated part of the system $V_H(t)$ is given by a measurement of this volume for certain temperature and by thermal expansion of the materials of the heated part (titanium for reservoir, stainless steel for capilary, see Section 4). The heat conductivity of titanium and stainless steel is large compared to water and therefore the temperature does not differ so much in various parts of the metals as can be also seen from the numerical simulations (Tab. 3). Therefore we consider the temperature in the titanium reservoir and in the steel capilary not a function of position in space. If we denote $T_R(t)$, resp. $T_C(t)$ the temperature in the titanium reservoir, resp. in capilary and we denote β_R and β_C volume thermal expansion coefficients of titanium and stainless steel at ambient temperature T_0 , we obtain

$$V_H(t) = V_R(T_0) \left(1 + \beta_R(T_R(t) - T_0) \right) + V_C(T_0) \left(1 + \beta_C(T_C(t) - T_0) \right)$$
(3.1.8)

where $V_R(T_0)$ and $V_C(T_0)$ are the volumes of water filled cavities inside the titanium reservoir (R) and inside the capilary (C) at temperature T_0 . These volumes will be known from differential mass measurements. $T_R(t)$ is measured by thermometer installed in a copper mounting attached to the titanium part and $T_C(t)$ should be with high accuracy the temperature of the thermal bath if the capilary is in direct contact with the thermal bath. Because the volume of the reservoir is larger compared to capilary, the second term will not be considered in this report.

3.2 General properties of the temperature distribution for the linear case

Now we will look to the temperature integrals in more detail. Since the temperature increase in the thermal bath is not far from linear function it is useful to study the behavior for the linear case.

Consider a system with heat conduction but without heat convection. Further, the temperature at the boundary of this system which is given by a function

$$T(t) = T_0 + \alpha t.$$
 (3.2.1)

Even if we have heat convection of the moving fluid this effect will have very small influence to the overall temperature distribution in the reservoir. Also the parts of the boundary of our system which are not in direct contact with the thermal bath are very small as compared to the rest (just the surfaces which are intersections of the water level in the bath with our system). We will now show some properties of the system assuming that it consists of one metarial . However, the result can be generalised to a system composed of several materials with continuous temperature and heat flux at their contact surfaces. The heat conduction equation has the form

$$\frac{\partial T}{\partial t} = \kappa \mathcal{L}(T) \tag{3.2.2}$$

where $\kappa = k/(\rho.C_p)$ (k is thermal conductivity of the material, ρ is its density and C_p is its heat capacity at constant pressure) and Δ is the Laplace operator. We look for a solution of the heat conduction equation (3.2.2) in the form (educated guess based on the numerical simulations)

$$T(x,t) = T_x(x) + \alpha t \tag{3.2.3}$$

where the index x denotes a spatial part of the temperature function. Inserting this function into equation (3.2.2) we find that it is a solution if the spatial part satisfies the equation

$$\mathcal{L}(T_x) = \frac{\alpha}{\kappa} \tag{3.2.4}$$

with boundary value of $T_x(x)$ equal to T_0 . In the numerical simulations we see that the temperature distribution approaches the form (3.2.3) after some time if the initial temperature is T_0 everywhere and the boundary temperature is given by the formula (3.2.1).

Intermezzo, if we know the solution T_{x1} of the Poisson equation (3.2.4) for certain value of $\alpha = \alpha_1$ then the solution T_{x2} for another value of $\alpha = \alpha_2$ and the same boundary condition $T_x = T_0$ is given as

$$T_{x2}(x) = \frac{\alpha_2}{\alpha_1} T_{x1}(x) + T_0 \left(1 - \frac{\alpha_2}{\alpha_1} \right)$$
(3.2.5)

as can be verified by direct examining of the boundary condition and inserting the solution into the equation (3.2.4).

Since the time evolution is linear everywhere in the heated part of the system according to (3.2.3) also for the function $T_M(t)$ we obtain

$$T_M(t) = T_x(x_M) + \alpha t \tag{3.2.6}$$

where $T_x(x_M)$ is the $T_x(x)$ function evaluated at the temperature measurement point. Using equations (3.1.1), (3.2.3) and (3.2.6) we get

$$\Delta T(x,t) = T_x(x) - T_x(x_M).$$
(3.2.7)

This implies that $\Delta T(x, t)$ does not depend on time! (This is confirmed by the numerical simulations, the third correction term in (3.1.7) goes to zero for increasing time.) Furthermore, it implies that using the formula (3.2.5) we obtain the following scaling properties for $\Delta T(x, t)$

$$\Delta T_2(x,t) = \frac{\alpha_2}{\alpha_1} \Delta T_1(x,t). \tag{3.2.8}$$

Now suppose that the temperature of the thermal bath is not exactly linear function of time. Consider that the temperature at the boundary of the heated part of our system is given as

$$T = T_0 + (\alpha + \Delta \alpha(t)).t.$$
(3.2.9)

The function $\Delta T(x, t)$ then can be written as

$$\Delta T(x,t) = \Delta T_x(x) + \Delta T_t(x,t)$$
(3.2.10)

where $\Delta T_x(x)$ is the function $\Delta T(x, t)$ how it would be if $\Delta \alpha(t) = 0$, i.e. in linear case, and $\Delta T_t(x, t)$ is a correction for nonlinearity. The function $\Delta T_x(x)$ satisfies the scaling law (3.2.8). For nearly linear temperature increase, i.e. $\Delta \alpha(t)$ small compared to α , the $\Delta T_t(x, t)$ function will be small compared to $\Delta T_x(x)$.

3.3 Numerical simulations for the temperature distribution

Simulations have been done for two reservoir geometries – one with volume of approx. 64 mm^3 (see Figure 2) and second with volume of approx. 1003 mm^3 (see Figure 6). The geometries were created according to drawings no. 120906-1 - 120906-5 of VSL. Basic dimensions, geometry for the simulation and mesh are depicted in Fig. 1-8.

For each geometry simulations have been done for four temperature boundary conditions (summarized in Tab. 1). Two (no. 1 and 2) correspond to a linear temperature increase of 0.01 K/s and 0.1 K/s. The other two (no. 3 and 4) correspond to a nonlinear temperature increase according to formulas in Tab. 1. These formulas are obtained from the requirement of a constant mass flowrate at the outlet,

assuming that the non homogeneous expansion coefficient and temperature increase can be neglected (hence, only the first term of (3.1.7) is considered). Note, this assumption turned out to be inaccurate for the larger temperature gradients (see next series of figures).

In table 1 the values of Q_m are the expected values of the mass flowrate and V are the reservoir volumes. The values of a and b are obtained from linear fit of a temperature derivative of water density as a function of temperature. The boundary condition no. 1 can be considered as linear approximation of boundary condition no. 3. And similarly the boundary condition no. 2 can be considered as linear approximation of the boundary condition no. 4. For a volume of 1000 mm³ and the third boundary condition, a flow rate of 120 nl/min should be obtained.

b.c. no.	formula	parameters	flowrate for 1000 mm ³
1	$T = T_0 + \alpha. t$	$\alpha = 0.01 K/s$	110 - 130
1			µg/min
2	$T = T_0 + \alpha. t$	$\alpha = 0.1 K/s$	1300 - 1700
Δ			µg/min
3	$T = T_0 - b/a + \sqrt{(b/a)^2 - 2Q_m/(Va).t}$	$Q_m/V = 0.0020 kg. m^{-3} s^{-1}$	120 μg/min
4	$T = T_0 - b/a + \sqrt{(b/a)^2 - 2Q_m/(Va).t}$	$Q_m/V = 0.025 kg. m^{-3} s^{-1}$	1500 µg/min
	$T_0 = 293.15 K, b/a = 21.77 K,$	$a = -0.00955 \ kg. \ m^{-3} K^{-2}$	

Tab. 1 Boundary conditions for temperature. The conditions b.c. 3 and b.c. 4 were formulated in order to obtain approximately constant mass flowrate Q_m which is given as the value of Q_m/V multiplied by the reservoir volume. Flowrate values for reservoir volume of 1000 mm³ are in the last column. The linear conditions 1 and 2 does not lead to constant flowrate but the b.c. 1 is similar to b.c.3 and leads to similar flowrates and b.c. 2 leads to similar flowrates as b.c. 4.

At the outlet from the capillary a zero gradient boundary condition for tempetaure was applied. For velocity field a noslip condition was applied at walls and fixed pressure condition was applied at the capillary outlet.



Fig. 1 Middle reservoir dimensions accrding to the drawing no. 120906-1.



Fig. 2 Geometry of the middle reservoir used for simulations.



Fig. 3 Mesh for the middle reservoir.



Fig. 4 Mesh for the middle reservoir - detail of capillary inlet.



Fig. 5 Dimensions of the large reservoir accrding to the drawing no. 120906-5.



× Zy

Fig. 6 Geometry of the large reservoir used for simulations.

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Fig. 7 Mesh for the large reservoir.



Fig. 8 Mesh for the large reservoir – detail of capillary inlet.

The aim of the simulations is to obtain the tempearture distribution in the reservoir as a function of time in order to be able to calculate the second and the third term of the formula (3.1.7). In the formula (3.1.7) the temperature T_M (*t*) measured by a thermometer inside the reservoir occurs. In the simulations this temperature was represented by a temperature at the inner wall of the reservoir in the point of the center of the end of stainless steel tube which contains the thermometer wires (points 1 in Fig. 15).

Tables for this temperature as a function of time were obtained for each simulation. Furthermore tables for average temperature $T_A(t)$ in the water part of a geometry as a function of time were obtained for each simulation. The average temperature is calculated as an integral of the temperature over the water volume devided by the water volume. The second term of (3.1.7) can then be expressed as

$$\int_{V_H(t)} \Delta T(x,t) dV = V_H(t) \cdot (T_A(t) - T_M(t)).$$
(3.3.1)

As discussed in Section 3.2, for a constant temperature gradient, the spatial temperature distribution can be described as:

$$\Delta T(x,t) = \Delta T_x(x) + \Delta T_t(x,t)$$
(3.2.10)

Therefore, an approximation for the average temperature, $T_A(t)$, is given as:

$$T_A(t) = c_1 T_M(t) + c_2 T_{copper}(t)$$

where T_{copper} (t) is the average temperature measured in the copper mounting blocks. Alternatively, the average temperature can be given as:

$$T_A(t) = T_M(t) + c$$

where c is constant in case of a constant temperature increase.

The simulations have been done with fixed reservoir geometry without thermal expansion of the reservoir walls. In this case the third term of (3.1.7) can be expressed as

$$\int_{V_{H(t)}} \frac{\partial \Delta T(x,t)}{\partial t} dV = \frac{\partial}{\partial t} \int_{V_{H}(t)} \Delta T(x,t) dV = V_{H} \frac{\partial}{\partial t} (T_{A}(t) - T_{M}(t)).$$
(3.3.2)

The time derivative has been derived numerically. Note, these correction terms can also be estimated for calibration work. The average temperature and time derivatives then follow from (a weighted) averaged of the installed temperature sensors.

Next the simulation results are presented. Graphs Fig. 9-11 represent the temperature distribution for the middle reservoir, boundary conditions no. 2 (see Tab. 1) and time 100 s. The temperature distribution for this case is typical for all simulated cases for the middle reservoir. The graphs for nonlinear cases do not differ much from their linear counterparts. Hence, the temperature increase is indeed not far from linear. The case with b.c. no. 1 differs from the case with b.c. no. 2 by temperature rescaling – the temperature scale is divided by 10 for b.c. no. 1. This corresponds to the scaling properties of temperature given by (3.2.8).

Graphs Fig. 12-14 represent the temperature distribution for the large reservoir, boundary conditions no. 2 and time 80 s. The temperature distribution for this case is typical for all simulated cases for the large reservoir similarly as for the case of the middle reservoir with the same scaling law.

Graphs Fig. 16-23 show temperature in points depicted in Fig. 15 as a function of time. These are three points selected for each reservoir size – point no.1 is representing the thermometer installation – i.e. the point where T_M is taken, point no.2 is the center of the reservoir and point no.3 is at the end of one of the capillaries.

Graphs Fig. 24-47 show how the particular terms of the formula (3.1.7) evolve in time for various cases. For each case three graphs are shown. The first graph (Fig. 24, 27, 30, 33, 36, 39, 42, 45) shows the first term of (3.1.7) and the sum of all three terms of (3.1.7) as a function of time. The second graph (Fig. 25, 28, 31, 34, 37, 40, 43, 46) shows the second term of (3.1.7) in % of the first term as a function of time. The third graph (Fig. 26, 29, 32, 35, 38, 41, 44, 47) shows the third term of (3.1.7) in % of the first term as a function of time.

The second and the third term of (3.1.7) show a damped oscilatory behaviour. The magnitude of these terms is significant for the flowrate determination with the required accuracy. For the cases with linear temperature increase the temperature difference $T_A(t) - T_M(t)$ oscilates around certain constant value and approaches this value with increasing time. Table 2 summarises some of the features of the evolution of the second and the third term of the formula (3.1.7). The quantities in the table 2 have the following meaning:

- t_{ex} ... times at which the oscilations have an extreme (first two deflection points (first derivative changes sign) are listed for the middle reservoir and only the first turning point is listed for the large reservoir)
- $Q2(t_{ex})$... value of the second term for $t = t_{ex}$ in % of the first term
- Q2(80s) ... value of the second term for t = 80 s in % of the first term
- ΔT_{av} (inf) ... the value which is approached by $T_A(t) T_M(t)$ for large times; for linear temperature increase the quantity $T_A(t) T_M(t)$ should converge to certain value which is in the table, for nonlinear increase the convergence is not ensured and a range of $T_A(t) T_M(t)$ is given in the table for range of times (40-80) s

- $Q3(t_{ex})$... value of the third term for t = t_{ex} in % of the first term
- Q3(80s) ... value of the third term for t = 80 s in % of the first term



Fig. 9 Temperature distribution for middle (64 mm³) reservoir, b.c. no. 2 (0.1 K/s) after 100 s. The black line is the (semi) axisymmetry line, the blue line is the transversal line.



Fig. 10 Temperature distribution for the middle reservoir, b.c. no. 2 (0.1 K/s) after 100 s – transversal line in the middle (64 mm³) of the cylinder.



Fig. 11 Temperature distribution for the middle (64 mm³) reservoir, b.c. no. 2 (0.1 K/s) after 100 s – axis of the cylinder. The apparent large osciliations in the middle part are most probably a numerical $\frac{1}{2}$



Fig. 12 Temperature distribution for the large reservoir (1003 mm³), b.c. no. 2 (0.1 K/s)and time 80 s. The black line is the (semi) axisymmetry line, the blue line is the transversal line.



Fig. 13 Temperature distribution for the large reservoir (1003 mm³), b.c. no. 2 (0.1 K/s)and time 80 s – transversal line in the middle of the cylinder.



Fig. 14 Temperature distribution for the large reservoir (1003 mm³), b.c. no. 2 (0.1 K/s)and time 80 s – axis of the cylinder.



Fig. 15 Points where temperature has been determined in more detail. Point 1 corresponds with the point where T_M is measured.



Fig. 16 Time evolution of temperature for the middle (64 mm³) reservoir and b.c. no. 2 (0.1 K/s). Red line is temperature at the point 1 (see Fig. 15), blue line at the point 2 and green line at the point 3 (blue and green are almost the same). Note that the maximum temperature difference corresponds with Figure 10 and is roughly 0.3 K.



Fig. 17 Time evolution of temperature for middle (64 mm³) reservoir and b.c. no. 4 (≈ 0.1 K/s). Blue line is temperature at the point 1 (see Fig. 15), red line at the point 2 and green line at the point 3 (red and green are almost the same). Note that this figure is similar to Figure 16, showing the temperature increase is indeed almost linear.



Fig. 18 Time evolution of temperature for middle (64 mm³) reservoir and b.c. no. 1 (0.01 K/s). Blue line is temperature at the point 1 (see Fig. 15), red line at the point 2 and green line at the point 3 (red and green are almost the same). Note that the maximum temperature difference corresponds with Figure 10 and is roughly 0.03 K, which is 1 tenth of the difference found for a temperature gradient of 0.1 K/s, proving that the temperature solutions can indeed be scaled.



Fig. 19 Time evolution of temperature for middle (64 mm³) reservoir and b.c. no. 3 (≈ 0.01 K/s). Blue line is temperature at the point 1 (see Fig. 15), red line at the point 2 and green line at the point 3 (red and green are almost the same).



Fig. 20 Time evolution of temperature for the large reservoir (1003 mm³)and b.c. no. 2 (0.1 K/s). Red line is temperature at the point 1 (see Fig. 15), blue line at the point 2 and green line at the point 3. Note that the larger reservoir results in larger temperature differences. The coldest point is found in center of the reservoir.



Fig. 21 Time evolution of temperature for the large reservoir (1003 mm³) and b.c. no. 4 (≈ 0.1 K/s). Red line is temperature at the point 1 (see Fig. 15), blue line at the point 2 and green line at the point 3.



Fig. 22 Time evolution of temperature for the large reservoir (1003 mm³) and b.c. no. 1 (0.01 K/s). Red line is temperature at the point 1 (see Fig. 15), blue line at the point 2 and green line at the point 3.



Fig. 23 Time evolution of temperature for the large reservoir (1003 mm³) and b.c. no. 3 (≈ 0.01 K/s). Red line is temperature at the point 1 (see Fig. 15), blue line at the point 2 and green line at the point 3.



Fig. 24 Term 1 and sum (true flowrate) of all three terms of the formula (3.1.7) as a function of time for middle (64 mm³) reservoir and b.c. no. 1 (0.01 K/s). See Figures 25 and 26 for the second and the third term (correction terms). The spikes are probably numerical artifacts.



Fig. 25 Term 2 (correction for spatial variation of the expasion coefficient) of the formula (3.1.7) as a function of time for middle (64 mm³) reservoir and b.c. no. 1 (0.01 K/s).



Fig. 26 Term 3 (correction for spatial variation of temperature gradient) of the formula (3.1.7) as a function of time for middle (64 mm³) reservoir and b.c. no. 1 (0.01 K/s). Correction term tends to zero for increasing time.



Fig. 27 Term 1 and sum (true flowrate) of all three terms of the formula (3.1.7) as a function of middle (64 mm³) for middle reservoir and b.c. no. 3 (≈ 0.01 K/s). See Figures 28 and 29 for the second and the third term (correction terms). Note that after, say, 1 minute the flow rate is fairly stable.



Fig. 28 Term 2 (correction for spatial variation of the expasion coefficient) of the formula (3.1.7) as a function of time for middle (64 mm³) reservoir and b.c. no. 3 (≈ 0.01 K/s). Note that the correction term is small enough to be neglected.



Fig. 29 Term 3 (correction for spatial variation of temperature gradient) of the formula (3.1.7) as a function of time for middle (64 mm³) reservoir and b.c. no. 3 (≈ 0.01 K/s). Note that the for t sufficiently large the correction term is small enough to be neglected.



Fig. 30 Term 1 and sum (true flowrate) of all three terms of the formula (3.1.7) as a function of time for middle (64 mm³) reservoir and b.c. no. 2 (0.1 K/s). See Figures 31 and 32 for the second and the third term (correction terms).



Fig. 31 Term 2 (correction for spatial variation of the expasion coefficient) of the formula (3.1.7) as a function of time for middle (64 mm³) reservoir and b.c. no. 2 (0.1 K/s).



Fig. 32 Term 3 (correction for spatial variation of temperature gradient) of the formula (3.1.7) as a function of time for middle (64 mm³) reservoir and b.c. no. 2 (0.1 K/s). Correction term tends to zero for increasing time.



Fig. 33 Term 1 and sum (true flowrate) of all three terms of the formula (3.1.7) as a function of time for middle (64 mm³) reservoir and b.c. no. 4 (≈ 0.1 K/s). See Figures 34 and 35 for the second and the third term (correction terms).



Fig. 34 Term 2 (correction for spatial variation of the expasion coefficient) of the formula (3.1.7) as a function of time for middle (64 mm³) reservoir and b.c. no. 4 (≈ 0.1 K/s).



Fig. 35 Term 3 (correction for spatial variation of temperature gradient) of the formula (3.1.7) as a function of time for middle (64 mm³) reservoir and b.c. no. 4 (≈ 0.1 K/s).



Fig. 36 Term 1 and sum (true flowrate) of all three terms of the formula (3.1.7) as a function of time for large reservoir (1003 mm³) and b.c. no. 1 (0.01 K/s). See Figures 37 and 38 for the second and the third term (correction terms).



Fig. 37 Term 2 (correction for spatial variation of the expasion coefficient) of the formula (3.1.7) as a function of time for large reservoir (1003 mm³) and b.c. no. 1 (0.01 K/s).



Fig. 38 Term 3 (correction for spatial variation of temperature gradient) of the formula (3.1.7) as a function of time for large reservoir (1003 mm³) and b.c. no. 1 (0.01 K/s). Correction term tends to zero for increasing time.



Fig. 39 Term 1 and sum (true flowrate) of all three terms of the formula (3.1.7) as a function of time for large reservoir (1003 mm³) and b.c. no. 3 (\approx 0.01 K/s). See Figures 40 and 41 for the second and the third term (correction terms).



Fig. 40 Term 2 (correction for spatial variation of the expasion coefficient) of the formula (3.1.7) as a function of time for large reservoir (1003 mm³) and b.c. no. 3 (≈ 0.01 K/s).



Fig. 41 Term 3 (correction for spatial variation of temperature gradient) of the formula (3.1.7) as a function of time for large reservoir (1003 mm³) and b.c. no. 3 (≈ 0.01 K/s).



Fig. 42 Term 1 and sum (true flowrate) of all three terms of the formula (3.1.7) as a function of time for large reservoir (1003 mm³) and b.c. no. 2 (0.1 K/s). See Figures 43 and 44 for the second and the third term (correction terms).



Fig. 43 Term 2 (correction for spatial variation of the expasion coefficient) of the formula (3.1.7) as a function of time for large reservoir (1003 mm³) and b.c. no. 2 (0.1 K/s).



Fig. 44 Term 3 (correction for spatial variation of temperature gradient) of the formula (3.1.7) as a function of time for large reservoir (1003 mm³) and b.c. no. 2 (0.1 K/s). Correction term tends to zero for increasing time.



Fig. 45 Term 1 and sum (true flowrate) of all three terms of the formula (3.1.7) as a function of time for large reservoir (1003 mm³) and b.c. no. 4 (≈ 0.1 K/s). See Figures 46 and 47 for the second and the third term (correction terms).



Fig. 46 Term 2 (correction for spatial variation of the expasion coefficient) of the formula (3.1.7) as a function of time for large reservoir (1003 mm³)and b.c. no. 4 (≈ 0.1 K/s).



Fig. 47 Term 3 (correction for spatial variation of temperature gradient) of the formula (3.1.7) as a function of time for large reservoir (1003 mm³) and b.c. no. 4 (≈ 0.1 K/s).

Tab. 2 Some features of the evolution of the terms in the formula (3.1.7). The meaning of the quantities is: t_{ex} ... times at which the oscilations have an extreme (first two turning points are listed for the middle reservoir and only the first turning point is listed for the large reservoir); $Q2(t_{ex})$... value of the second term for $t = t_{ex}$ in % of the first term; Q2(80s) ... value of the second term for $t = t_{ex}$ in % of the first term; Q2(80s) ... value of the second term for t = 80 s in % of the first term; ΔT_{av} (inf) ... the value which is approached by $T_A(t) - T_M(t)$ for large times, for linear temperature increase the quantity $T_A(t) - T_M(t)$ should converge to certain value which is in the table, for nonlinear increase the convergence is not ensured and a range of $T_A(t) - T_M(t)$ is given in the table for range of times (40-80) s; $Q3(t_{ex})$... value of the first term. The quantities with asterix goes to zero for large time. The listed times of extremes are more or less the same if we take term 2 and term 3 in absolute units or in % of term 1. The only exception is marked in red colour – in this case the function in absolute units was used to determine the time of

maximum.

	Term 2			Term 3					
	t _{ex}	$Q2(t_{ex})$	Q2(80s)	ΔT_{av} (inf)	t _{ex}	$Q3(t_{ex})$	Q3(80s)	Q2(80s)+Q3(80s)	
	s	%	%	K	S	%	%	%	
Mid hal	18	-0.11	0.001	0.019	30	2.03	0 10 [*]	0.080	
Mid bei	53	-0.090	-0.091		60	-0.50	0.18	0.089	
Mid ha?	18	-0.11	0.096	0.017-	30	2.06	0.12	0.044	
Mild DCS	58	-0.084	-0.080	0.018	65	-0.54	0.15	0.044	
Mid bo?	18	-0.98	0.6	0.19	40	1.3	-0.20*	0.90	
Mid bc2	70	-0.61	-0.0		70	-0.23		-0.80	
Mid bo4	11	-1.1	0.52	0.17 –	30	3.6	15	0.07	
Mild 0C4	50	-0.62	-0.55	0.18	57	-0.82	1.3	0.97	
Large bc1	35	-0.38	-0.34	0.07	55	2.4	0.8^{*}	0.46	
Large bc3	35	-0.37	-0.32	0.07	55	2.9	1.4	1.1	
Large bc2	32	-3.1	-2.2	0.7	55	2.7	0.9*	-1.3	
Large bc4	26	-3.4	-2.0	0.6 - 0.8	55	6.2	1.8	-0.2	

3.4 Temperature distribution in metal parts

For each simulation tables of minimal temperature as a function of time were obtained for each particular material of the system. For copper, titanium and stainless steel parts a maximal temperature is the one at the outer boundary. From the knowledge of maximal and minimal temperatures the maximal temperature difference $\Delta T_{max} = T_{max} - T_{min}$ was calculated in each particular material. For linear temperature increase this temperature difference approaches certain constant value. These values are listed in table 3 below.

	$\Delta T_{max}(K)$					
	copper	titanium	steel			
Mid b.c. 1	0.0012	0.010	0.041			
Mid b.c. 2	0.012	0.10	0.41			
Large b.c. 1		0.0063	0.041			
Large b.c. 2		0.063	0.41			

Tab. 3 Temperature differences in metal parts

We see that in the copper and titanium parts the temperature distribution is almost homogeneous.

3.5 Conclusions on thermal expansion term

As discussed earlier, the second term of the formula (3.1.7) represents a contribution of nonhomogeneity of the thermal expansion coefficient $\partial \rho / \partial T$. The third term of this formula represents a contribution of non-homogeneity of temperature increase. From the simulations it follows that these terms are significant for the total mass flow rate, especially for a large temperature increase and low starting temperature. The third correction term can be neglected for almost linear temperature gradient and stabilisation time which is large enough (several minutes). The second correction term can be reduced by starting from a higher temperature. However, durint the start up phase both terms are too large to be discarded.

Hence, if a flowrate with stability below several tenths of percent is needed within 60 s, a bathtemperature as a function of time would have to be determined from further computations. Linear temperature increase or temperature increase calculated from the requirement of stability of the first term of (3.1.7) does not give a stable flowrate with required accuracy within the period of one minute. Determination of the bath-temperature increase for stable flowrate would be probably easier if the stabilisation time would be longer – e.g. several minutes. In this case the oscilations would be already damped enough. Since the calibration times will be in the order of 5 minutes, the determination of bath-temperature increase is not expected to be a major problem.

The results obtained here were verified also for coarser computational mesh in case of the middle reservoir and b.c. no. 2 with results not differing significantly. Hence, one could argue the global values are mesh converged. However, the numerical artifacts shown may be due to a poor or too low grid resolution. Refining the grids in these areas may change the solution.

4 Thermal expansion of the reservoir walls

The second term in (2.4) describes thermal expansion of the reservoir and the heated part of the capilary. A density of water which appears in the second term of (2.4) is a density at the boundary between water and the wall. Consider the temperature at the wall in form

$$T(x,t) = T_R(t) + \Delta T_R(x,t)$$
(4.1)

where $T_R(t)$ is the temperature as measured by the thermometer installed in the copper mounting. The $\Delta T_R(x,t)$ deviation should be small as compared to $T_R(t)$. Estimation of its value can be done based on the numerical simulations. The density at the wall is given as

$$\rho(T(x,t)) = \rho(T_R(t) + \Delta T_R(x,t)) = \rho(T_R(t)) + \frac{\partial \rho}{\partial T}(T_R(t)) \cdot \Delta T_R(x,t)$$
(4.2)

where we neglect the second and higher order terms. The second term of (2.4) then can be written as

$$\int_{\partial V_H(t)} \rho(x,t)\vec{\xi}(x,t)d\vec{S} = \rho(T_R(t)) \int_{\partial V_H(t)} \vec{\xi}(x,t)d\vec{S} + \frac{\partial\rho}{\partial T}(T_R(t)) \int_{\partial V_H(t)} \Delta T_R(x,t)\vec{\xi}(x,t)d\vec{S}.$$
(4.3)

Using (3.1.8) we obtain

д

$$\int_{V_H(t)} \vec{\xi}(x,t) d\vec{S} = \frac{dV_H(t)}{dt} = V_R(T_0)\beta_R \frac{dT_R(t)}{dt} + V_C(T_0)\beta_C \frac{dT_C(t)}{dt}.$$
(4.4)

So in total we have

$$\int_{\partial V_{H}(t)} \rho(x,t)\vec{\xi}(x,t)d\vec{S}$$

$$= \rho(T_{R}(t)) \cdot \left(V_{R}(T_{0})\beta_{R}\frac{dT_{R}(t)}{dt} + V_{C}(T_{0})\beta_{C}\frac{dT_{C}(t)}{dt}\right)$$

$$+ \frac{\partial\rho}{\partial T}(T_{R}(t)) \cdot \int_{\partial V_{H}(t)} \Delta T_{R}(x,t)\vec{\xi}(x,t)d\vec{S}.$$
(4.5)

From a simulation we can obtain an upper bound for $\Delta T_R(x, t)$. Consider that $|\Delta T_R(x, t)| < \Delta T_{Rmax}$. Then the upper bound for the second term in (4.5) is

$$\left|\frac{\partial\rho}{\partial T}(T_{R}(t))\int_{\partial V_{H}(t)}\Delta T_{R}(x,t)\vec{\xi}(x,t)d\vec{S}\right| < \left|\frac{\partial\rho}{\partial T}(T_{R}(t))\Delta T_{Rmax}\cdot\frac{dV_{H}(t)}{dt}\right|.$$
(4.6)

From the graphs Fig. 16-23 we see that the temperature difference between points 1 and 3 (see Fig. 15 for the point definitions) is below 0.5 K for the b.c. no. 2 and 4 and below 0.05 K for b.c. no. 1 and 3. If we consider this as the maximal difference ΔT_{Rmax} we obtain that the second term of (4.6) is not larger then 0.015 % of the first term in case of b.c. no. 2 and 4 and not larger then 0.0015 % of the first term of (4.6) is therefore negligible and we can write

$$\int_{\partial V_H(t)} \rho(x,t)\vec{\xi}(x,t)d\vec{S} = \rho(T_R(t)) \cdot \left(V_R(T_0)\beta_R \frac{dT_R(t)}{dt} + V_C(T_0)\beta_C \frac{dT_C(t)}{dt}\right).$$
(4.7)

5 Cooling

The third term in (2.4) describes the part of mass flow generated by water density changes in the cooling part of the capilary.

5.1 Physical model

The capilary is inserted into a hose with streaming water. The cooling water enters the hose with ambient temperature. The temperature of water in the cooling capilary reach the ambient temperature after some length so it is reasonable to consider the temperature of water as

$$T(x,t) = T_0 + \Delta T_C(x,t).$$
(5.1.1)

For the derivative of density with respect to time we can write

$$\frac{\partial \rho}{\partial t}(x,t) = \frac{\partial \rho}{\partial T} \left(T(x,t) \right) \frac{\partial T(x,t)}{\partial t} = \left(\frac{\partial \rho}{\partial T} (T_0) + \frac{\partial^2 \rho}{\partial T^2} (T_0) \cdot \Delta T_C(x,t) \right) \frac{\partial T(x,t)}{\partial t}.$$
(5.1.2)

For the third term in (2.4) we then obtain

$$\int_{V_{C}(t)} \frac{\partial \rho(x,t)}{\partial t} dV = \frac{\partial \rho}{\partial T}(T_{0}) \int_{V_{C}(t)} \frac{\partial T(x,t)}{\partial t} dV + \frac{\partial^{2} \rho}{\partial T^{2}}(T_{0}) \int_{V_{C}(t)} \Delta T_{C}(x,t) \frac{\partial T(x,t)}{\partial t} dV.$$
(5.1.3)

At first we will do some analytical estimations and then we will proceed to numerical results. In our analytical estimate we will consider that the flow inside the capilary is slow enough such that the convection effects are unimportant.

Consider a cylinder which is a piece of the capilary. The thermal energy increase in the cylinder equals to the heat transfered to the cylinder through its wall. It is described by an equation

$$\frac{d}{dt} \int_{V} c_p \rho T dV = \int_{\partial V} k. \, gradT d\vec{S}.$$
(5.1.4)

We will be especially interested in the longitudinal temperature distribution in the capilary and therefore we split the integration into longitudinal and transversal part. We introduce a coordinate x in the longitudinal direction which runs from 0 to L in our cylinder and we get

$$\frac{d}{dt} \int_{0}^{L} \left(\int_{S} c_{p} \rho T dS \right) dx = \int_{S} k \cdot \frac{\partial T}{\partial x} dS \mid_{x=L} - \int_{S} k \cdot \frac{\partial T}{\partial x} dS \mid_{x=0} + 2\pi r \int_{0}^{L} k \frac{\partial T}{\partial n} dx$$
(5.1.5)

where the surface integral on the right hand side were split into the integral over the bottom part, up part and the wall of the cylinder, the derivative of temperature with respect to *n* denotes the derivative along the normal to the wall of the cylinder and *r* denotes the capilary radius. The values of c_p , ρ and *k* have constant values in stainless steel and different constant values in water. However surface of water in the cut through the cylinder is only about 0.4% of the total surface of the cut so we will neglect it and consider the material parameters constant and the same everywhere. If we take the average temperature in the cut

$$\overline{T}(x) = \frac{1}{S} \int_{S} T dS$$
(5.1.6)

where *S* is the surface area of the cut then (5.1.5) gives

$$c_p \rho S \frac{d}{dt} \int_0^L \bar{T} \, dx = k S \frac{\partial \bar{T}}{\partial x} |_{x=L} - k S \frac{\partial \bar{T}}{\partial x} |_{x=0} + 2\pi r \int_0^L k \frac{\partial T}{\partial n} dx.$$
(5.1.7)

The first two terms on the right hand side can be writen as

$$kS\frac{\partial\bar{T}}{\partial x}|_{x=L} - kS\frac{\partial\bar{T}}{\partial x}|_{x=0} = kS\int_{0}^{L}\frac{\partial^{2}\bar{T}}{\partial x^{2}}dx.$$
(5.1.8)

If we insert it into (5.1.7) and we consider that the equation holds for arbitrary long cylinder then we can remove the integrals to obtain

$$c_p \rho S \frac{\partial \bar{T}}{\partial t} = kS \frac{\partial^2 \bar{T}}{\partial x^2} + 2\pi r k \frac{\partial T}{\partial n}.$$
(5.1.9)

The second term on the right hand side of the equation (5.1.9) is basically a heat flux density through the wall of the cylinder. Let us suppose that the heat flux density through the cylinder wall is proportional to the difference between the average temperature in the capilary and the average temperature outside the capilary which is the ambient temperature T_0 . Then we can write

$$\frac{2\pi r}{c_p \rho S} k \frac{\partial T}{\partial n} = -\gamma (\bar{T} - T_0)$$
(5.1.10)

where γ is a positive constant. The equation (5.1.9) then gives

$$\frac{\partial \bar{T}}{\partial t} = \kappa \frac{\partial^2 \bar{T}}{\partial x^2} - \gamma (\bar{T} - T_0)$$
(5.1.11)

where

$$\kappa = \frac{k}{c_p \rho}.$$
(5.1.12)

We now consider the longitudinal coordinate x to have its origin at the beginning of the cooled part of the capilary. We look for a solution of the equation (5.1.11) with linearly increasing temperature at the origin and vanishing derivative of the temperature far from the origin, i.e. we consider the following boundary conditions

$$\overline{T}(x=0) = T_0 + \alpha t, \qquad \frac{\partial \overline{T}}{\partial x}(x \to \infty) = 0.$$
 (5.1.13)

A hint from numerical simulation is that the solution depends linearly on time (with high degree of accuracy) in every position but the rate of temperature change differs place to place. We therefore look for a solution in form

$$\overline{T}(x,t) = a(x)t + b(x).$$
 (5.1.14)

This leads to a pair of differential equations

$$\kappa \frac{d^2 a}{dx^2} - \gamma a = 0, \qquad \kappa \frac{d^2 b}{dx^2} - \gamma b = a - \gamma T_0. \tag{5.1.15}$$

If we apply an initial condition $\overline{T}(x, 0) = T_0$ to the formula (5.1.14) we obtain $b(x) = T_0$ but in this case the equations (5.1.15) lead to a solution a(x) = 0 and therefore $\overline{T}(x, t) = T_0$. If we do not apply the initial condition but just the boundary conditions (5.1.13) we obtain the following solution

$$\overline{T}(x,t) = T_0 + \alpha e^{-\sqrt{\frac{\gamma}{\kappa}}x} \left(t - \frac{x}{2\sqrt{\kappa\gamma}}\right).$$
(5.1.16)

We should understand the formula (5.1.16) as a temperature wave which propagates along the capilary with speed of $2\sqrt{\kappa\gamma}$ and disturbes the original state $\overline{T}(x,0) = T_0$. Therefore we apply the formula (5.1.16) for $x < 2\sqrt{\kappa\gamma} t$ and for $x \ge 2\sqrt{\kappa\gamma} t$ we have $\overline{T}(x,t) = T_0$. It seems to be a reasonable assumption that the temperature of water inside the capilary is more or less the same as the temperature of the capilary itself at a given distance from the inlet and therefore is also given by the formula (5.1.16). We will verify this assumption by comparison of the formula (5.1.16) with results of numerical simulations for the temperature distribution inside the capilary.

5.2 Numerical simulations for the cooling term

Simulations have been done with a capilary of outer diameter of 1.58 mm, inner diameter of 0.1 mm and length of 15 cm. The capillary is made of stainless steel with thermal conductivity of 16 W/(m.K), density of 8030 kg/m³ and thermal capacity of 500 J/(kg.K). The capilary is inserted to a cooling tube with flowing water. The inner diameter of the cooling tube is 6.4 mm. The cooling water enters the

cooling tube from the opposite side than the water from the reservoir. The flowrate of the cooling water is between 13 mL/min and 1300 mL/min. This corresponds to a velocity range of 0.0067 m/s to 0.67 m/s. The simulations have been done for flowrates corresponding to reservoir volumes of 100, 1000 and 10000 mm³, temperature increase rates of 0.01 K/s and 0.1 K/s and cooling flowrates of 13 mL/min and 1300 mL/min.

Boundary conditions:

Inlet to the capilary: a constant velocity of water, temperature increasing in time (same as the thermal bath temperature)

Outlet from the capilary: a fixed pressure, zero normal temperature derivative

Steel cut at the inlet: temperature increasing in time (same as the thermal bath temperature)

Steel cut at the outlet: zero normal temperature derivative

Inlet to the cooling pipe (opposite side then the inlet to the capillary): constant velocity of the cooling water, constant temperature (same as the ambient temperature)

Outlet from the cooling pipe: fixed pressure, zero normal temperature derivative

Wall of the cooling pipe: noslip velocity condition, thermal insulation

The COMSOL file with the computation settings has a name cooling.mph.

The mesh used for this computation is depicted in Fig. 48.

In Fig. 49 we can see temperature isolines in a cut of the cooling pipe for temperature increase $\alpha = 0.1$ K/s, cooling flowrate $Q_C = 1300$ mL/min, time t = 100 s and capillary flowrate 180,4 nL/min (inlet velocity of 0.38 mm/s) corresponding to reservoir volume 100 mm³. In Fig. 50 we can see a temperature distribution along the inner capillary wall for various times and for the same conditions as above. Fig. 51 shows a comparison of temperatures at the inner wall of the capillary and at the axis of the capillary (i.e. in the middle of the water channel). From the graphs we can see that the temperature decreases rapidly with a distance from the capillary inlet. We can also see that for the capillary flowrate 180,4 nL/min the temperature does not change significantly in the crossection of water channel inside the capillary. Graphs for a situation with $\alpha = 0.01$ K/s instead of $\alpha = 0.1$ K/s look similarly – just with the temperature scale divided by 10.

Graphs Fig. 52-54 show the same quantities as above only with minimal cooling of $Q_c = 13$ mL/min instead of maximal cooling of $Q_c = 1300$ mL/min. We can observe a smaller temperature gradient in the cooling water near the inlet part of the capillary and we can see that the capillary is cooled down to the ambient temperature at a longer distance which is still quite short (will be quantified bellow).

Graphs Fig. 55-56 show temperature isolines and comparison of temperatures at inner capillary wall and axis for temperature increase $\alpha = 0.1$ K/s, cooling flowrate $Q_C = 1300$ mL/min, time t = 100 s and capillary flowrate 1804 nL/min (inlet velocity of 3.83 mm/s) corresponding to reservoir volume 1000 mm³.

Graphs Fig. 57-58 show the same quantities for capillary flowrate 18036 nL/min (inlet velocity of 38.3 mm/s) corresponding to reservoir volume 10000 mm^3 .

In these graphs we can see how the temperature isolines in the water channel inside the capillary change with increasing flowrate. We can also observe that the temperature distribution at the inner wall of the capillary almost does not depend on the capillary flowrate whereas the temperature distribution at the water channel axis depends on the flowrate – the higher is the flowrate the larger is the shift of the temperature curve to the higher values of distance from the capillary inlet.



Fig. 48 Mesh for cooling computations. From left is a ractangle corresponding to the water chanel inside the capillary, the capillary itself and the cooling water.



Fig. 49 Temperature isolines for $\alpha = 0.1$ K/s, $Q_C = 1300$ mL/min, t = 100s and flow velocity corresponding to reservoir volume 100 mm³.



Fig. 50 Temperature at wall of the water channel inside the capillary as a function of distance from the origin (the distance is in meters) for $\alpha = 0.1$ K/s, $Q_C = 1300$ mL/min and flow velocity corresponding to reservoir volume 100 mm³. Curves for times 0 – 90s with step of 10 s.



Fig. 51 Temperature at wall (green) and at axis (blue) of the water channel inside the capillary as a function of distance from the origin (the distance is in meters) for $\alpha = 0.1$ K/s, $Q_C = 1300$ mL/min, t = 100s and flow velocity corresponding to reservoir volume 100 mm³.



Fig. 53 Temperature at wall of the water channel inside the capillary as a function of distance from the origin (the distance is in meters) for $\alpha = 0.1$ K/s, $Q_C = 13$ mL/min and flow velocity corresponding to reservoir volume 100 mm³. Curves for times 0 – 90s with step of 10 s.



Fig. 54 Temperature at wall (green) and at axis (blue) of the water channel inside the capillary as a function of distance from the origin (the distance is in meters) for $\alpha = 0.1$ K/s, $Q_C = 13$ mL/min, t = 100s and flow velocity corresponding to reservoir volume 100 mm³.



Fig. 55 Temperature isolines for $\alpha = 0.1$ K/s, $Q_C = 1300$ mL/min, t = 100s and flow velocity corresponding to reservoir volume 1000 mm³. Colors are suppressed.



Fig. 56 Temperature at wall (green) and at axis (blue) of the water channel inside the capillary as a function of distance from the origin (the distance is in meters) for $\alpha = 0.1$ K/s, $Q_C = 1300$ mL/min, t = 100s and flow velocity corresponding to reservoir volume 1000 mm³.



Fig. 57 Temperature isolines for $\alpha = 0.1$ K/s, $Q_C = 1300$ mL/min, t = 100s and flow velocity corresponding to reservoir volume 10000 mm³. Colors are suppressed.



Fig. 58 Temperature at wall (green) and at axis (blue) of the water channel inside the capillary as a function of distance from the origin (the distance is in meters) for $\alpha = 0.1$ K/s, $Q_C = 1300$ mL/min, t = 100s and flow velocity corresponding to reservoir volume 10000 mm³.

Now we will verify the analytical formula (5.1.16) by comparing it with the numerical data. There is one unknown parameter γ in the formula. The parameter κ is calculated from stainless steel properties and its value is $\kappa = 3.985 \text{ mm}^2/\text{s}$. We will obtain the value of γ by fitting the formula (5.1.16) to the numerical data. More precisely we will make an exponential fit of the derivative of temperature at the inner wall of the capillary with respect to time at a time t = 98 s. According to (5.1.16) this derivative should be

$$\frac{dT}{dt} = \alpha e^{-\sqrt{\frac{\gamma}{\kappa}}x}.$$
(5.2.1)

From the fit we obtain the value of γ and then we can evaluate deviations of the theoretical formula (5.1.16) from the numerical data at various times and positions inside the capillary.

The fits for various parameters are depicted in graphs Fig. 59-64. The values of $\sqrt{\gamma/\kappa}$ and γ are summarised in table 4 below for various parameters. We see that the values of γ are very similar for a given value of cooling flowrate, i.e. γ significantly depends only on the cooling flowrate. This is what we expect since γ is a proportionality coefficient between the tempearture difference capillary - ambient and heat flux from the capillary to the ambient.

The table 4 also describes deviations of numerical data from the analytical formula. There are maximal deviations of temperature itself and also of its time derivative. There are maximal deviations at inner wall of the capillary and at the axis. Values for various times are listed. The maximal deviations of temperature are in % of the difference $T(x) - T_0$ and the maximal deviations of temperature derivatives are in % of dT/dt. The deviation's maxima are taken from a capillary part of length of 5 mm in case of maximal cooling and length of 10 mm in case of minimal cooling. The values in red color for the minimal cooling are taken from a length of 5 mm since the percentual deviations are increasing further but the the temperature difference $T(x) - T_0$ is already so small that the deviations are not significant in its absolute value.

Further discussion can be found behind the table 4.



Fig. 59 Exponential fit of temperature derivative with respect to time at the inner capillary wall at t = 98 s for $\alpha = 0.1$ K/s, $Q_C = 1300$ mL/min and flow velocity corresponding to reservoir volume 100 mm³.



Fig. 60 Exponential fit of temperature derivative with respect to time at the inner capillary wall at t = 98 s for $\alpha = 0.1$ K/s, $Q_C = 13$ mL/min and flow velocity corresponding to reservoir volume 100 mm³.



Fig. 61 Exponential fit of temperature derivative with respect to time at the inner capillary wall at t = 98 s for α = 0.01 K/s, Q_C = 1300 mL/min and flow velocity corresponding to reservoir volume 100 mm³.



Fig. 62 Exponential fit of temperature derivative with respect to time at the inner capillary wall at t = 98 s for $\alpha = 0.01$ K/s, $Q_C = 13$ mL/min and flow velocity corresponding to reservoir volume 100 mm³.



Fig. 63 Exponential fit of temperature derivative with respect to time at the inner capillary wall at t = 98 s for $\alpha = 0.1$ K/s, $Q_C = 1300$ mL/min and flow velocity corresponding to reservoir volume 1000 mm³.



Fig. 64 Exponential fit of temperature derivative with respect to time at the inner capillary wall at t = 98 s for $\alpha = 0.1$ K/s, $Q_C = 1300$ mL/min and flow velocity corresponding to reservoir volume 10000 mm³.

	γ	γ		Max. deviation of		Max. deviation of			
	$\sqrt{\kappa}$	-		Т			dT/dt		
	1/mm	1/s		%	of (T – '	T ₀)	% of dT/dt		
			t =	10 s	50 s	98 s	10 s	50 s	98 s
$V = 100 \text{ mm}^3$, $k = 0.1 \text{ K/s}$	1 200	6 676	wall	8.6	8.3	8.0	8.6	8.0	7.6
$Q_C = 1300 \text{ mL/min}$	1.290	0.030	axis	9.0	8.8	8.4	9.1	8.4	7.9
$V = 100 \text{ mm}^3$, $k = 0.1 \text{ K/s}$	0 5 9 7	1 270	wall	1.8	2.1	2.0	2.5	2.1	1.7
$Q_{\rm C} = 13 \text{ mL/min}$	0.587	1.372	axis	-3.4	2.3	2.1	2.7	2.2	1.8
$V = 100 \text{ mm}^3$, $k = 0.01 \text{ K/s}$	1 202	6 5 5 0	wall	8.0	8.0	8.0	8.1	8.0	8.0
$Q_{\rm C} = 1300 \; {\rm mL/min}$	1.282	0.330	axis	8.1	8.1	8.1	8.2	8.1	8.1
$V = 100 \text{ mm}^3$, $k = 0.01 \text{ K/s}$	0.592	1 254	wall	-1.9	2.0	2.1	2.2	2.2	2.1
$Q_C = 13 \text{ mL/min}$	0.385	1.554	axis	-5.4	2.1	2.2	2.3	2.3	2.2
$V = 1000 \text{ mm}^3$, $k = 0.1 \text{ K/s}$	1 270	6510	wall	8.6	8.4	8.0	8.7	8.0	7.6
$Q_{\rm C} = 1300 \; {\rm mL/min}$	n 1.279	0.519	axis	11.6	11.4	11.0	11.7	11.0	10.4
$V = 10000 \text{mm}^3$, $k = 0.1 \text{ K/s}$	1 250	6 227	wall	10.2	9.9	9.5	10.2	9.4	8.9
$Q_C = 1300 \text{ mL/min}$	= 1300 mL/min 1.250	0.227	axis	35	34	34	35	34	33

Tab. 4 Values of coeffitients obtained from exponential fits and maximal deviations of the analytical formula from numerical data.

5.3 Conclusions on effect of cooling

From the table 4 we see that the values obtained from numerical simulation are in satisfactory agreement with the values obtained by analytical estimate besides the situation with the largest reservoir volume 10000 mm³ which in fact will not be realised anyway. Assuming a temperature distribution according to formula (5.1.16) which changes only in longitudinal direction inside the capilary we have a maximal error of around 10 % in every situation.

If we use the formula (5.1.16) to evaluate the contribution to mass flow (the third term in (3.1.7)) we obtain

$$\int_{V_{C}(t)} \frac{\partial \rho(x,t)}{\partial t} dV = \alpha S \sqrt{\kappa/\gamma} \left(\frac{\partial \rho}{\partial T}(T_{0}) + \frac{\partial^{2} \rho}{\partial T^{2}}(T_{0}) \frac{1}{2} \alpha \left(t - \frac{1}{4\gamma} \right) \right)$$
(5.3.1)

where S is the crossection of the water channel inside the capillary. Coming to formula (5.1.3) we made the following approximations $(1 - e^{-2\gamma t}) \approx (1 - e^{-4\gamma t}) \approx 1$ which are well satisfied after several seconds of evolution. We can introduce an effective cooling volume and effective cooling expansion factor as

$$V_{Ceff} = S\sqrt{\kappa/\gamma} , \qquad B_{Ceff} = \left(\frac{\partial\rho}{\partial T}(T_0) + \frac{\partial^2\rho}{\partial T^2}(T_0)\frac{1}{2}\alpha\left(t - \frac{1}{4\gamma}\right)\right). \tag{5.3.2}$$

Then we have

$$\int_{V_C(t)} \frac{\partial \rho(x,t)}{\partial t} dV = \alpha V_{Ceff} B_{Ceff}.$$
(5.3.3)

The value of effective cooling length $\sqrt{\kappa/\gamma}$ is around 0.8 mm for the strongest cooling and around 1.7 mm for the weakest cooling as we can calculate from the values in table 4. The capilary diameter is 0.1 mm so we obtain $V_{Ceff} = 0.006 \ mm^3$ for the strongest cooling and $V_{Ceff} = 0.013 \ mm^3$ for the

weakest cooling. If we look to the formula (3.1.7) we see that for a linear temperature increase the main part of the mass flow (the first term) is given as

$$\frac{dm}{dt} = \alpha V_H \frac{\partial \rho}{\partial T} (T_M) \tag{5.3.4}$$

where V_H is the volume of the heated part of the system. The contribution of cooling to the mass flowrate therefore is

$$\frac{Q_C}{Q} = \frac{\alpha V_{Ceff} B_{Ceff}}{\alpha V_H \frac{\partial \rho}{\partial T} (T_M)} \approx \frac{V_{Ceff}}{V_H}.$$
(5.3.5)

In table below we express the contribution of cooling to the flowrate in percents.

$V_H (\mathrm{mm}^3)$	$Q_C = 1300 \text{ mL/min}$	$Q_C = 13 \text{ mL/min}$
17	0.035 %	0.076 %
63	0.0095 %	0.021 %
1003	0.0006 %	0.0013 %

Tab. 5 Percentual part of mass the flowrate generated in the cooling pipe.

The flowrate contribution coming from a thermal expansion of the cooled part of the capillary which is given by the fourth term in the formula (3.1.7) is considered negligible.

6 Conclusions

Five basic components of flowrate have been identified. The main one (first term of (3.1.7)) can be calculated from measured temperature inside the reservoir as a function of time, from known reservoir volume and from known water properties (temperature dependence of density). The other components are – a) correction due to inhomogeneity of thermal expansion coefficient of water (second term of (3.1.7)) which is directly connected to inhomogeneity of temperature in the reservoir, b) correction due to thermal expansion of reservoir walls and d) correction due to the cooling process outside the thermal bath. The corrections a) and b) have been modeled numerically and have been identified as significant contributions to the flowrate. These corrections have to be taken into account also when we want to determine the evolution of temperature in the thermal bath which leads to a stable flowrate. The correction c) was described by an analytical formula. The correction d) has been modeled numerically and has been identified as not so important and negligible as compared to the other contributions.