

## **CFD and Tracer Experiments**

### **Part I. Residence Time Distribution**

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#### Summary:

This article concerns evaluation of RTD (Residence Time Distribution) of continuous apparatuses either experimentally or by numerical simulation. Questions about reliability of CFD (Compute Fluid Dynamics) predictions and verification are discussed. Experimental verification of CFD results can be based upon comparison of impulse responses (RTD). This procedure has been demonstrated on analysis of continuous direct ohmic heater. It was very surprising, but the RTD of ohmic heater calculated by pretty complicated 3D model (program Fluent) did not agree with experiments even for extremely fine computational mesh. Experiments were repeated for different concentrations of tracer (KCl) giving the same responses measured by conductivity probes, and therefore the experimental results can be considered as reliable. Failure of Fluent is probably caused by difficulties in describing details of cross flow through small slots in electrodes (characteristic dimension 2 mm) and the bulk flow within the heater (characteristic dimension hundreds mm). Surprisingly, very simple and only two-dimensional model was able to describe the impulse response fairly well. The most important geometrical parameter (width of perforation of electrodes) had to be considered as a free parameter of model, identified by comparison of impulse response with experiment. However, optimal value of this parameter is close to the actual width, and therefore the simple 2D model seems to be a better description of flow field, than the complicated 3D model.

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## 1. Introduction

Most of processes in apparatuses of chemical and food industries are continuous and stationary. Performance, intensification and quality improvement of these processes can be studied using models, which are always based on the flow pattern description. Velocity field inside apparatuses can be identified numerically (CFD) or for example by experimental tracer techniques. CFD programs like Fluent, CFX, Cosmos,... can simulate tracer experiments, thus helping in their preparation. The two following approaches are currently used:

- Calculation of stationary velocity field and then evaluation of particle trajectories (Lagrangian approach). This procedure is suitable for simulation of experiments monitoring single particle motion.
- Calculation of stationary velocity field and *transient* field of either temperature or concentration. The time course of temperature/concentration at inlet is specified as either unit step or a short pulse, which corresponds to tracer experiments for evaluation washing function or residence time distribution (impulse response).

CFD simulation of processes offer solutions, which should be verified experimentally, because CFD is nothing else than a model, based upon many hypothesis and simplifications. Suitable tool for verification is stimulus-response method using radioisotopes as tracers. Simplest stimulus response method is restricted to observation of input/output signals (concentrations of tracer or even temperature if the thermal diffusivity equals molecular diffusivity). In the case, that the stimulus function is a very short pulse, the detected response is directly proportional to the RTD.

## 2. CFD modelling of tracer experiment

Numerical modeling and experiments are tested on continuous **direct ohmic heater**, shown in Fig.4. The reason why this continuous heater has been selected for tracer experiments

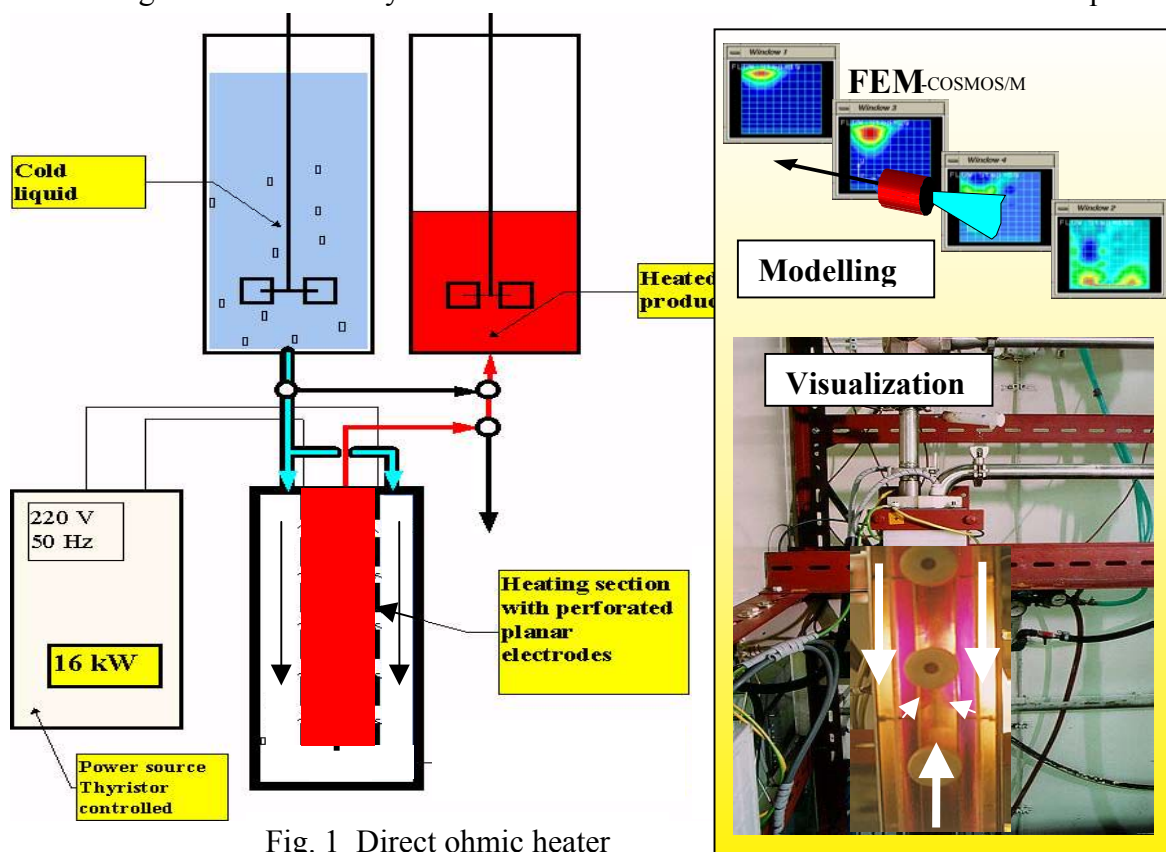


Fig. 1 Direct ohmic heater

lies in the fact, that the flow pattern – counter current parallel flows – is frequently encountered in apparatuses (not only heat exchangers but also for example core annulus flow pattern in cracking units).

Numerical modeling has been performed using CFD programs COSMOS (Finite Elements) and FLUENT (Control Volumes). It is interesting to mention the amount of data processed by Fluent: 600000 nodal point, 100 time steps. Connectivity matrix, table of coordinates of nodal points and first of all concentrations in all nodes and in all time steps of simulation fill two CD-ROMs (approx. 1 GB)! Enormous requirements follow from the fact, that the Fluent was used for modeling of cross-flow through perforated electrodes and the size of control volumes was determined by the size of small slits.

In the case, when electrodes are impermeable flat plates, the model of geometry is much simpler, and the Cosmos Explorer (limited version of a general purpose FEM program) can be used. First the simple two-dimensional solution was calculated, see Fig.4.

Three-dimensional case is similar, only the run time is much longer. In view of symmetry of the flow pattern it is sufficient to calculate the velocities and temperatures in only one quarter of a heating tank, see simplified geometry in Fig.5. The problem was formulated as transient laminar flow of a Newtonian liquid

$$\rho=1000 \text{ kg/m}^3$$

$$c_p=4200 \text{ J/(kg.K)}$$

$$\lambda=0.6 \text{ W/(m.K)}$$

$$\mu=1 \text{ Pa.s}$$

Velocity profile was considered constant at inlet  $u_y=0.03 \text{ m/s}$ . Cross section area of a quarter of inlet channel is  $A_{in}=0.02 \times 0.03=6 \cdot 10^{-4} \text{ m}^2$  and volumetric flowrate through the heater is 72 ml/s. Reynolds number at lateral channel is  $Re_1=0.6$  (mean velocity 0.021 m/s) and  $Re_2=1.3$  in the central channel (mean velocity 0.027 m/s). It follows that even for water having viscosity 1000 times smaller, the flow will be laminar.

Cosmos cannot solve problems with mixtures (water + tracer), however the movement of tracer can be simulated by movement of temperature field. Stimulus function is an approximation of short pulse, see Fig. 5, time course of temperature prescribed at the inlet (uniform injection across the whole cross section is assumed). Duration of pulse is 3 s. Estimating internal volume of heater to 3.8 l, the mean residence time is approximately 53 seconds. It means that the duration of stimulus functions is approx. 5 % of mean residence time at the selected flowrate 72 ml/s. Though the time of experiment is usually recommended to be three times the mean residence time, numerical solution has been performed at time range of only 0 – 80 seconds. Results confirmed that this time span is sufficient for evaluation of most important

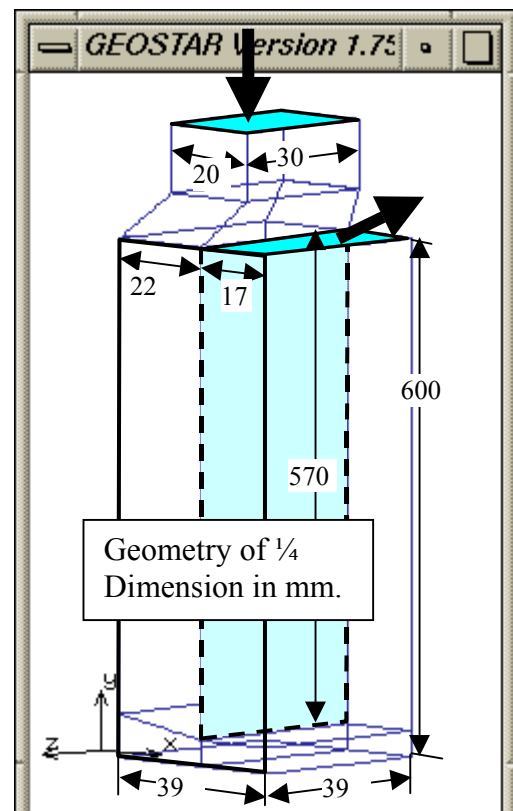


Fig.2 Geometry of heating vessel (1/4)

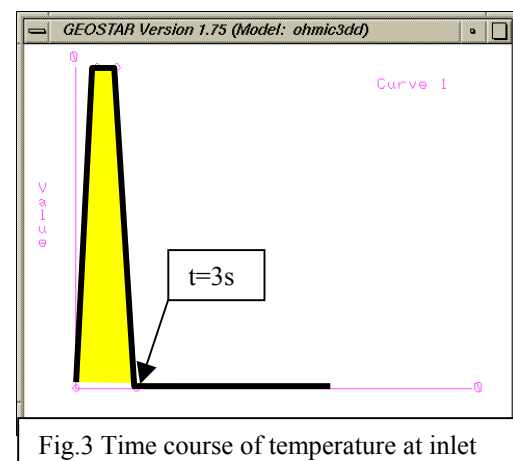


Fig.3 Time course of temperature at inlet

phenomena, see Fig.7. It is seen that the peak of temperature arrives to the bottom of vessel at approximately 20 seconds, and then rises upwards. What is remarkable: Even if the boundary condition at a symmetry plane prescribes zero heat flux, the maximum temperature is not located at the center.

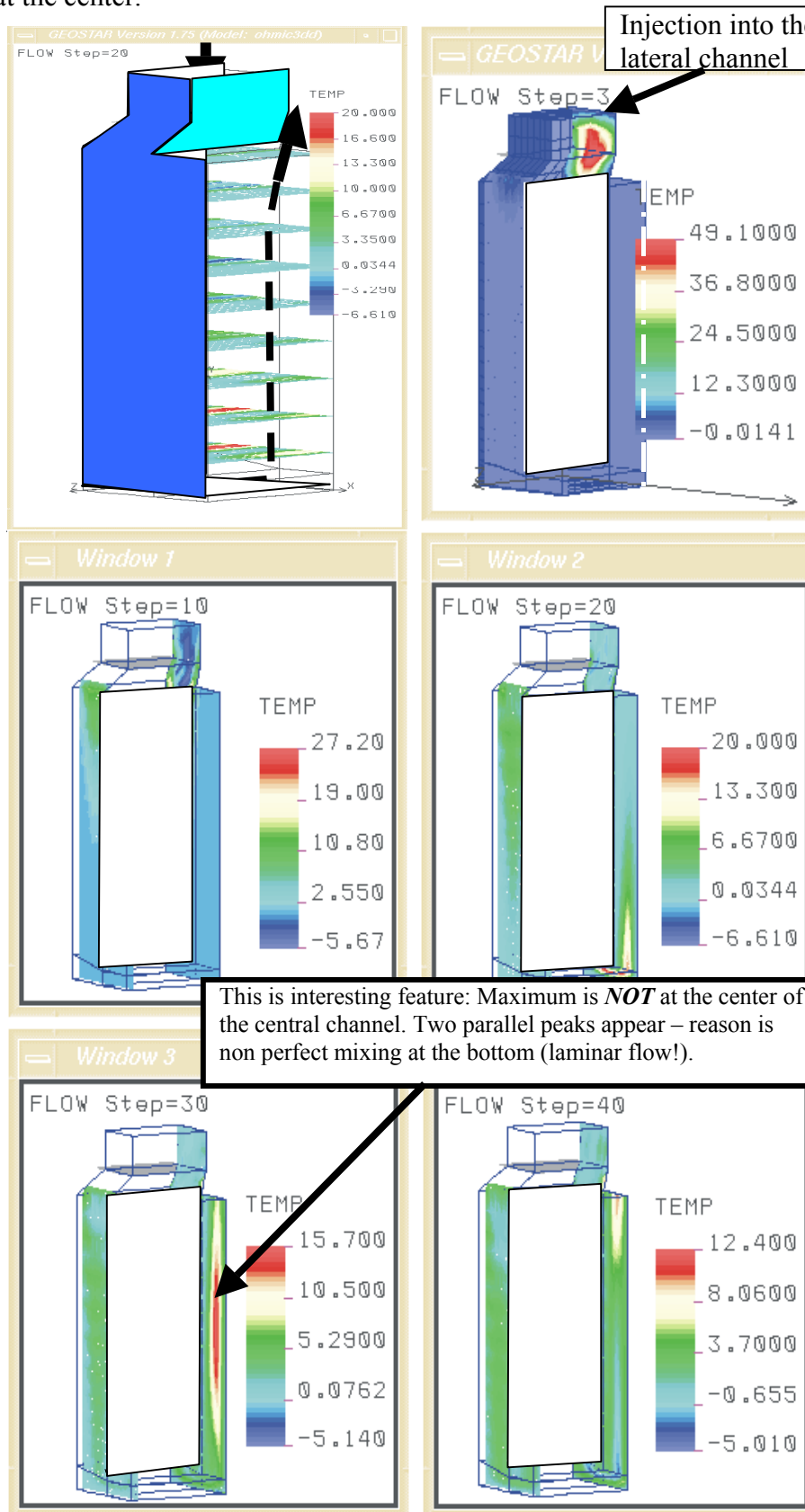


Fig.4 Numerical prediction of temperature profiles at t=3,10,20,40 seconds.

Results predict existence of two spatial maximums at a given cross-section profile within the heating zone between electrodes. This prediction can be easily explained: Streamlines at a symmetry plane correspond to particles, which were near the outer wall in lateral channels, and therefore are delayed. This phenomenon need not be true in reality, because the CFD model assumes perfectly symmetric flow and does not take into account any irregularity of geometry and natural convection.

### 3. Residence time distribution

Assuming that the stimulus function (see Fig.3) is a good approximation of  $\delta$ -function, the residence time distribution is given by response at outlet, calculated as average concentration/temperature at the exit cross section of the central channel

$$c_{out}(t) = \frac{\int_S u(x,z)c(t,x,z)dx dz}{\dot{V}} \quad (1)$$

This time course is reproduced by the detector located at the outlet stream only in the case, that the stream is well mixed. If this requirement is not met, the response corresponds to the mean concentration at exit

$$c_{out}^S(t) = \frac{\int_S c(t,x,z)dx dz}{S} \quad (2)$$

The time courses calculated according to Eqs. (1), (2) using velocity and temperature profiles predicted by COSMOS, are presented in Fig.5.

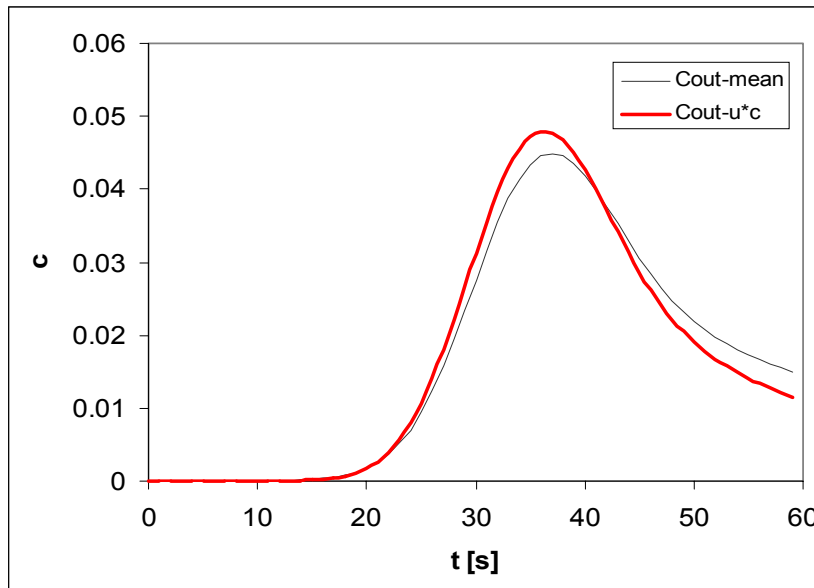


Fig.5 Responses at exit cross section calculated as integrals of calculated profiles  $c(t,x,z)$ .

It is obvious, that the difference is not negligible, however the characteristic shape of RTD obtained by using either (1) or (2) is preserved.

## 4. Experiments

Experimental measurement of RTD by conductivity method used a KCl solution as a tracer. Experimental set-up is in Fig.6.

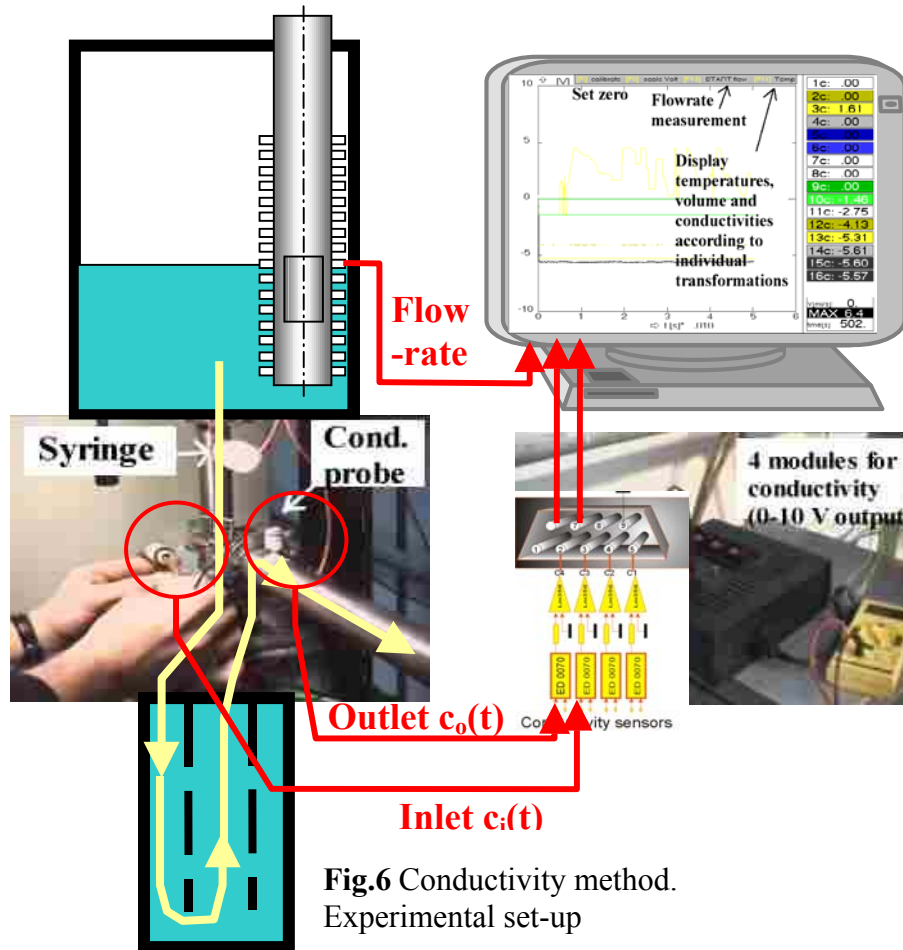


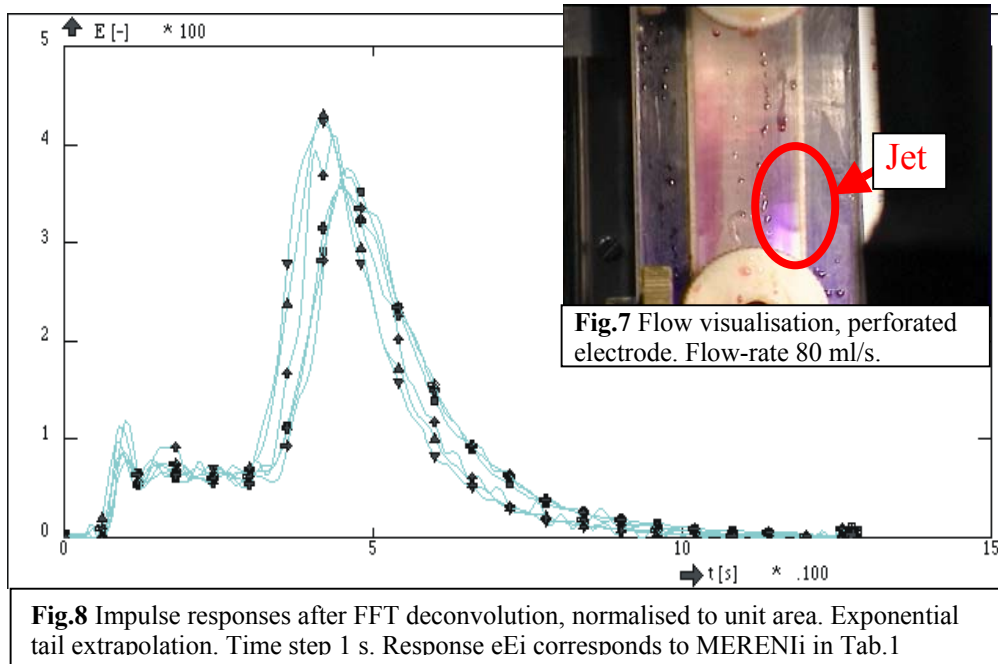
Fig.6 Conductivity method. Experimental set-up

Limited number of experiments has been done with the aim to verify the influence of gravity flow if the density of tracer is different than the density of water.

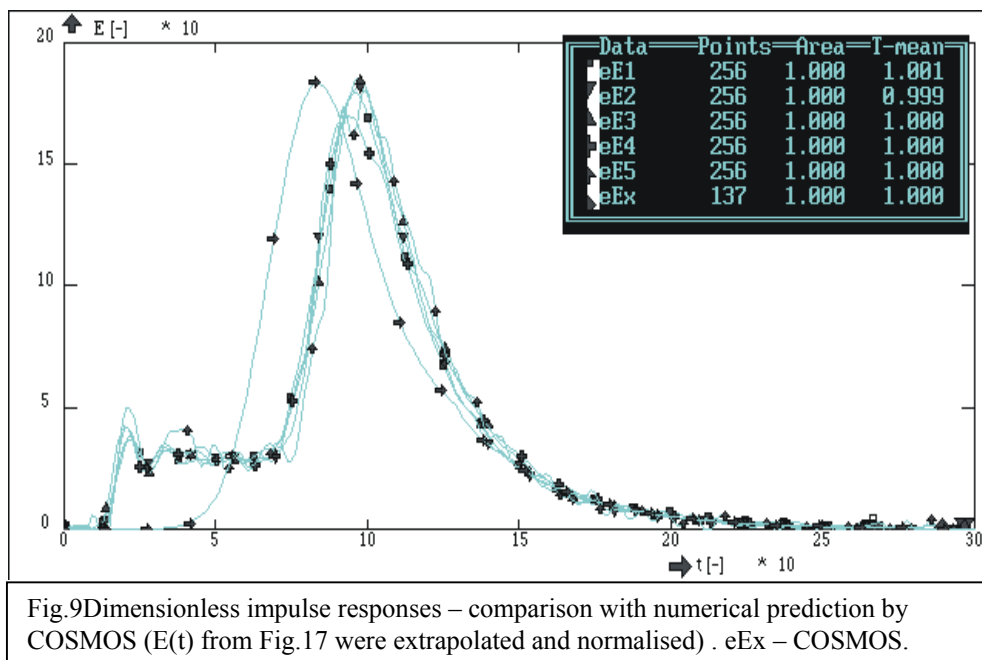
Tab.1 (source of experimental data Kareš (1999))

Experiment	Tracer KCl	Flowrate	T [C]	t-mean [s]	$\sigma^2$ [-]	t-first [-]
MERENI1	C+56.5g/l	82.4	14	48.14	0.147	0.13
MERENI2	C+56.6g/l	80	13.4	42.95	0.144	0.13
MERENI3	56.5 g/l	89.4	13	43	0.138	0.13
MERENI4	56.5 g/l	91	12	47.8	0.14	0.13
MERENI5	28.25 g/l	89	12.2	44.1	0.147	0.13
MERENI6	28.25 g/l	78	12.2	47.7	0.15	0.13
<b>COSMOS</b>		72		<b>43.48</b>	<b>0.109</b>	<b>0.4</b>
<b>FLUENT</b>		40		<b>155 (tail)</b>	<b>0.568</b>	<b>0.1</b>

Experiments used  $\text{KMnO}_4$  (potassium permanganate) as a colour marker, and visualisation confirmed previously obtained results: cross-flow through the slits of perforated electrode has character of a jet, penetrating into the main stream, see Fig.7. This cross-flow explains the initial plateau region of impulse response, see Fig.8.



Because the COSMOS model was designed for impermeable electrodes, the theoretical impulse response is different and does not predict this initial jump effect, see Fig.9.



Therefore it can be concluded that at a range of high Reynolds numbers (approx. 700) the perforation worsens the residence time distribution. This is confirmed also by numerical values of variance and by the low values of the first appearance time in Tab.1. However, it is believed, that at a regime of creeping flow, the jets will be suppressed and the RTD characteristic will be improved. The positive information concerns the methodology of experiments: It seems that the influence of gravity flow due to different density of tracer is negligible (mass fractions of KCl in water solution 0.056 and 0.028).



## 5. Experiments and identification of CFD model

Results of numerical simulations presented in Ch.2, corresponding to the flow within the heater equipped by full electrodes cannot be compared with previous experiment.

Flow pattern in the heater was analysed also by FLUENT, Zajíček (1999), and unlike the simplified geometry used in the COSMOS model, all details of perforation of electrodes was considered, see Fig. 10.

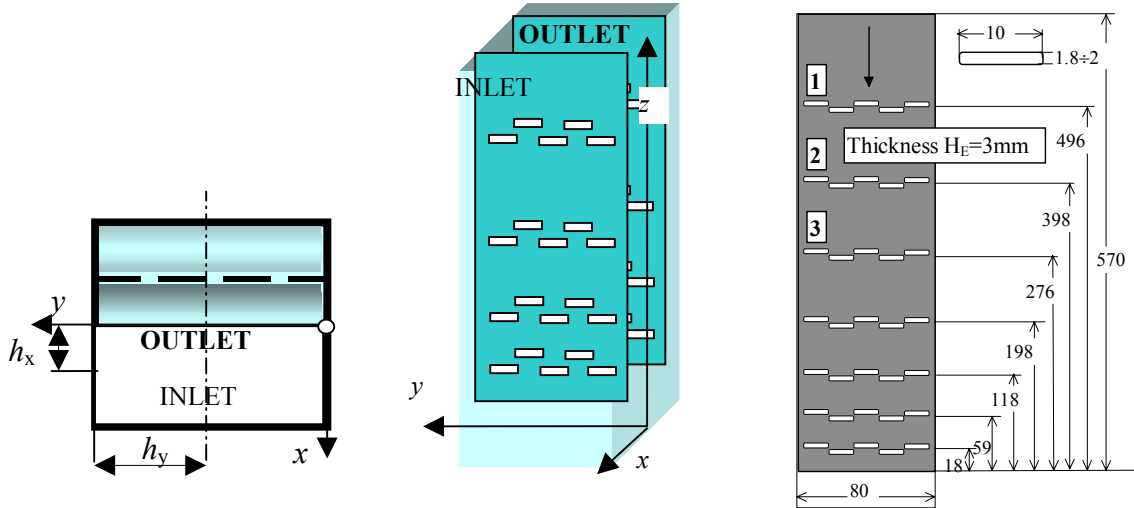


Fig.10 Geometrical model FLUENT. Geometry of perforated electrode.

This model has 614348 nodal points (approximately hundred times more than COSMOS). FLUENT calculated evolution of concentration field of the water 2, replacing initial content of heater (water 1) during 178 seconds from start up flow at a constant flow-rate 40 ml/s (constant time steps 2 seconds). In order to calculate the response according to Eq.(1) it is necessary to know the velocity profile at the outlet. Unfortunately this information is missing in ref. Zajicek (1999). Therefore it was assumed that the flow is fully developed at outlet, and the velocity profile was approximated by

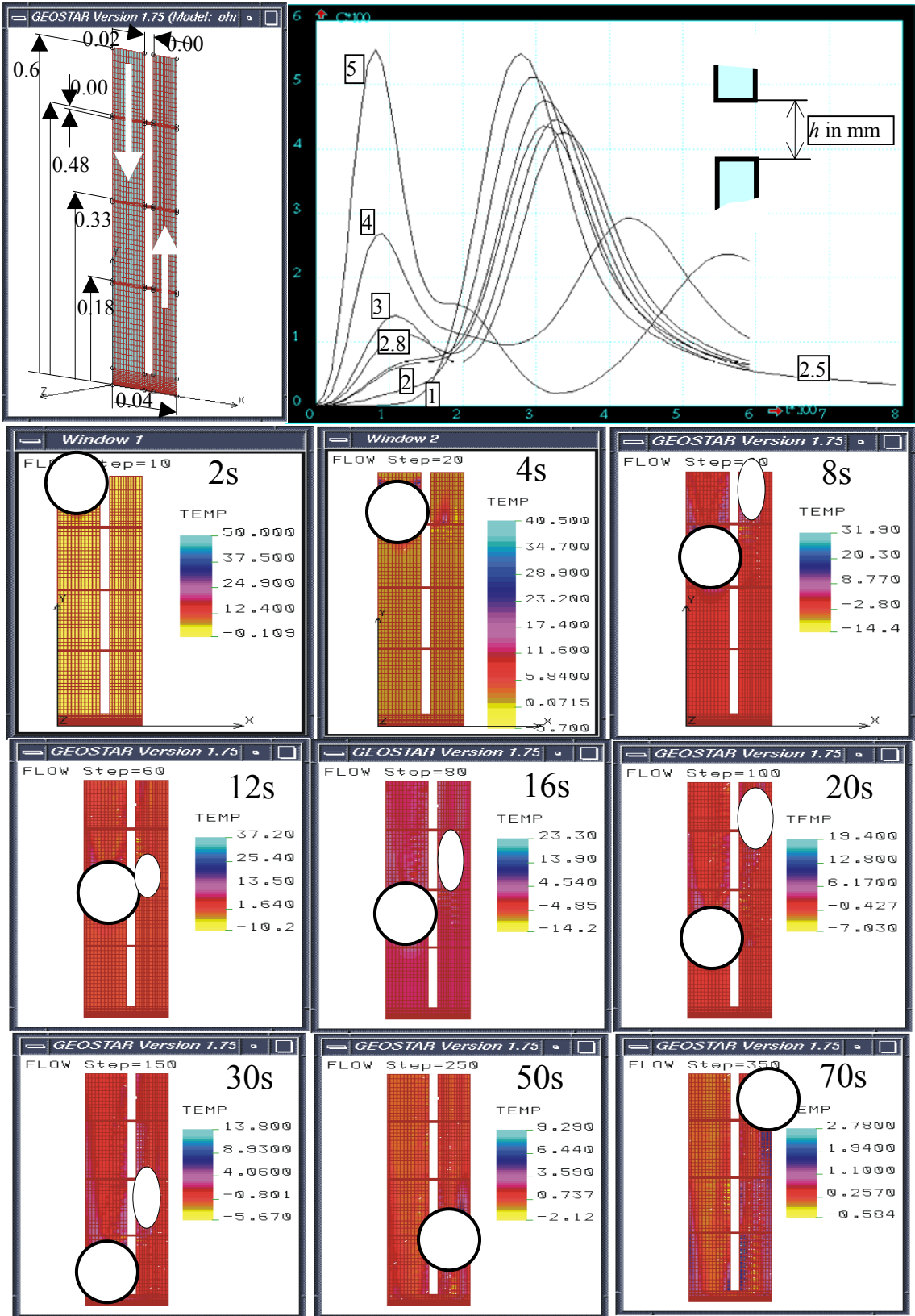
$$w(x, y) = \frac{9\dot{V}}{16h_x h_y} \left[ 1 - \left( \frac{x}{h_x} \right)^2 \right] \left[ 1 - \left( \frac{y}{h_y} - 1 \right)^2 \right] \quad (3)$$

The only difference between the FLUENT model and experiments, was flowrate. Example calculated by FLUENT assumed volumetric flowrate 40 ml/s, that is nearly two times less than in experiment or COSMOS modelling. Another difference had been in the form of stimulus function: It was not a pulse but a step function 0 – 1, and corresponding response is therefore integral distribution function  $F(t)$ . However, it is easy to transform the integral distribution into the impulse response, and result is presented in Fig.13. RTD calculated by FLUENT is obviously far from experimentally observed courses  $E(t)$ , see also Tab.1. This discrepancy cannot be explained only by different flowrates. It seems that the numerical prediction of the cross-flow through perforated electrodes is overestimated, and even if the numerical mesh is very fine and the flow regime is laminar, the numerical solution is quite unacceptable (though at a first glance it seems to be perfect).

This example demonstrates problems encountered in using CFD programs even in seemingly easy situations (laminar flow). The problems arise from the fact that the CFD model tries to describe relatively large region (height of vessel 0.6 m) and at the same time details describing flow within a narrow gap (0.002 m) – therefore the density of mesh is changing more than hundred times. In this case it is more effective to use only 2 dimensional models, see



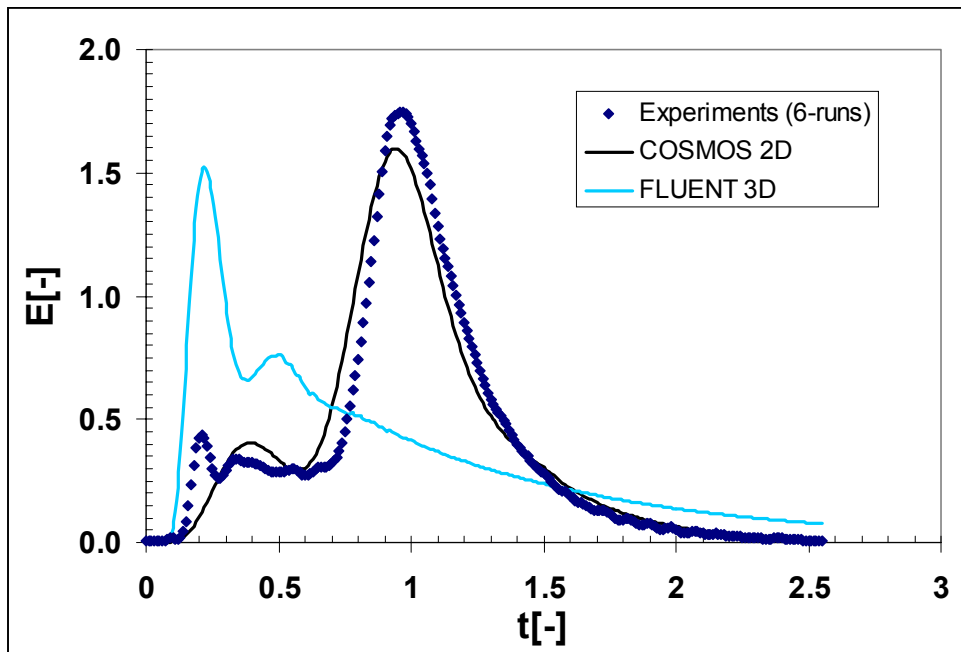
extremely simplified geometry in Fig.11. This figure demonstrates a typical time evolution of temperature field, corresponding to a pulse stimulus function (short temperature pulse at inlet). Effect of cross flow is clearly seen.



**Fig.11** Simplified 2D geometry, impulse responses for  $h=1,2,2.5,2.8,3,4,5$  mm, velocity 0.03 m/s. Isotherms at 2 to 70 seconds (for thickness of gap  $h=3$ mm)

It is not possible to expect fully realistic description of flow field using such a simplified model. However, some geometrical characteristic can be considered as free parameters, which can be identified by comparison numerical prediction and experimental impulse responses. The width of gaps in perforation  $h$  has been selected as the free parameter and several runs were performed for  $h=1,2,2.5,2.8,3,4,5$  mm (actual width was approximately 2 mm). Resulting responses calculated from outlet profiles of temperature and velocity according to Eq.(1) are presented also in Fig. 11.

A high sensitivity of the RTD shape upon the parameter  $h$  enables fitting "by eyes". The width  $h=0.0025$  has been selected as the best result, and normalised RTD response is compared with experimental data and with the prediction by 3D Fluent model in Fig.12.



**Fig.12** Dimensionless residence time distributions. Experimental course is average of 6 experiments (Fig.21), COSMOS 2D model having 600 elements, and  $h=0.028$  m (2% time delay was added – substitution of inlet section), FLUENT more than 600000 nodes.

It is obvious, that the simple 2D model predicts the RTD much better than the extremely large 3D model.

## **7. Conclusions:**

It is often believed that the expanding applications of CFD (numerical experiments) make the real experiments obsolete and redundant. However, even such flows, which can be completely mathematically described (e.g. laminar flows using Navier Stokes equations) can be difficult for CFD modelling and it is not easy to verify correctness of prediction. Experimental verification can be based upon comparison of impulse responses (RTD). It was very surprising, but RTD calculated by extremely fine mesh (Fluent) predicted quite different course (and even the shape) than experiments. Experiments used KCl solution as a tracer and the concentration response was measured by conductivity probes. Experiments were repeated for different concentrations of tracer at the same flowrate (80 ml/s) and because all responses and identified RTD were nearly the same, the experiment can be considered as reliable. Failure of Fluent could be ascribed to the different flowrates (40 ml/s in model, and 80 ml/s in experiment) nevertheless this explanation is improbable, because results were converted to dimensionless form, independent of flowrate. Surprisingly, very simple and only two-dimensional model was

able to describe the impulse response rather well. The most important geometrical parameter (width of perforation of electrodes) had to consider as a free parameter, identified by comparison of impulse response with experiment. However, optimal value of this parameter is close to the actual width, and therefore the simple 2D model can be a better description of flow field, than the complicated 3D model.

### List of symbols

$c$	concentration of tracer	[kg.m <sup>-3</sup> ]
$c_{out}$	concentration of tracer at output	[kg.m <sup>-3</sup> ]
$E$	residence time distribution (impulse response)	[-]
$S$	surface	[m <sup>2</sup> ]
$t$	time	[s]
$T$	temperature	[°C]
$u, v, w$	velocity componetnts	[m.s <sup>-1</sup> ]
$V$	volume	[m <sup>3</sup> ]
$\dot{V}$	volumetric flowrate	[m <sup>3</sup> .s <sup>-1</sup> ]
$x, y, z$	coordinates of cartesian system	[m]
$\mu$	viscosity	[Pa.s]
$\rho$	density	[kg.m <sup>-3</sup> ]

### References

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