

CFD simulation of homogenisation time measured by radiotracers*

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Abstract A methodology for CFD (Computational Fluid Dynamics) simulation of radiotracer experiments was suggested. The most important parts of the methodology for validation of CFD results by radiotracers are: a) successful simulation of tracer experiment by CFD code (numerical solution of tracer dispersion in a stirred tank), which results in tracer concentration field at several time intervals; b) post-process data treatment, which uses detection chain description and which enables to simulate the detector measurement of homogenisation time from the tracer concentration field evaluated by CFD code.

Key words liquid mixing • homogenisation time • radiotracer • CFD simulation • detection chain response

The detected tracer concentration is given by

$$N(t, x', y', z') = \iiint_V D(x, y, z) c(t, x, y, z) dx dy dz,$$

where $c(t, x, y, z)$ is the distribution of the tracer concentration in the tank volume V obtained from CFD calculations; $D(x, y, z)$ is the transfer (weight) function of radiotracer detection and x', y', z' describe position of the detector. Two ways of evaluation were suggested for $D(x, y, z)$ function: 1) by using algorithms for collimated detectors; 2) by interpolation of values representing the detector response to a point source situated inside a tank.

Numerical simulation of homogenisation time by CFD for different values of detected volume was confronted with measurement of homogenisation time by a conductivity probe and using the following radioisotopes: ^{198}Au , ^{82}Br and ^{24}Na . A simple detection algorithm called 'view factor' was successfully tested in the CFD simulation of homogenisation time, which was measured with ^{198}Au as a tracer. A simple simulation of homogenisation time for different radiotracers (on the basis of tracer concentration calculated by CFD for several positions in front of the collimated aperture of the detector and on the basis of PSR (Point Source Response) measurement in the same positions) was compared with tracer experiments with acceptable agreement.

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Introduction

Results of continuous measurement of homogenisation time of liquid in a stirred tank depend on the scale of scrutiny [11]. Experimental techniques use the probe, which is situated inside the tank, such as the conductivity method, or outside of the tank as in the case of gamma-radiotracer methods. Expected value of homogenisation time for a given degree of homogenisation is higher when using the conductivity method because the conductivity probe measures a relatively small volume in contrast to application of radiotracer, when the volume is much greater. Measurement through the wall of the tank is a great advantage of the radiotracer application, but a comparison of these results with another method requires determination of the measured volume, which is not easy. Simulation of measurement by CFD code can help to solve the problem.

Numerical simulation of liquid homogenisation in mechanically stirred vessels is rather complicated and mostly experimental verification is needed. There is no problem to perform experiments in a laboratory, when it is possible to use transparent equipment walls or when the probes can be situated inside the vessel. However, the probes situated inside the vessel can influence velocity field – especially in the case of homogenisation of liquid with high viscosity. Sometimes the use of the probe inside the industrial equipment is difficult or even not possible. In this case, gamma radiotracers are used, which enable to follow the tracer concentration by detectors situated outside the vessel. The tracer concentration depends on the size and position of the volume, which is “seen” by the detectors. This volume depends on the detection system and also on the gamma radiotracer, which is used for the homogenisation analysis [10]. A radiotracer with high gamma ray energy is measured from the depth of the vessel greater than in the case of a tracer with low energy. CFD evaluation of velocity field and concentration distribution was performed using a commercial software FLUENT 6.1 in a way similar to that was already used and published by several authors (e.g. [1]).

FLUENT 6.1 was used for simulation of liquid homogenisation in the mixed vessel with a Rushton turbine. Numerical CFD simulation of homogenisation time for different values of detected volume was confronted with measurement of homogenisation time using the conductivity probe and also using the radioisotopes $K^{198}Au(CN)_2$, ^{82}BrK and $^{24}NaCl$. Detected size of the tank volume was affected by energy of the radioisotope used.

Measurements of homogenisation time in a mixed vessel

Homogenisation analysis of water was performed in a cylindrical vessel (see Fig. 1a), (with diameter $T = 0.2$ m, height $H/T = 1$, with four baffles, width $0.1T$), equipped with the standard Rushton turbine, which was centrally situated in the vessel with a position from the bottom $h/D = 1$. Another important dimensions of the impeller: diameter $D/T = 0.30$, blade height $/D =$

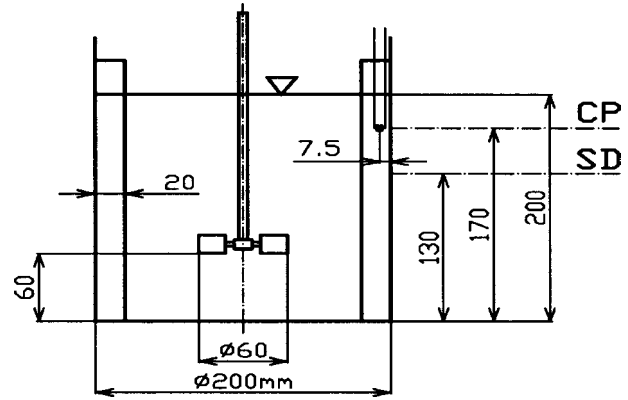


Fig. 1a. Cylindrical vessel with Rushton turbine.

0.20 and length/ $D = 0.25$, with disk diameter $d/D = 0.75$. Position of conductivity probe (CP) and scintillation detector (SD) is shown in Fig. 1a as well.

Intensity of mixing is evaluated from homogenisation time suitably read off from the registered response to instantaneous dosing of small amounts of tracer to the system. The degree of inhomogeneity is given by the formula:

$$(1) \quad \xi = \frac{|N^*(t) - N_\infty^*|}{|N_\infty^* - N_b^*|},$$

where: $N^*(t)$ is the count rate registered at time t ; N_∞^* is the count rate after complete homogenisation; N_b^* is the background count rate.

Evaluation of homogenisation time is clearly visible in Fig. 1b.

The read off homogenisation time will be probably shorter than homogenisation time obtained by the conductivity method. The difference is caused by the fact that when measuring with radioisotopes, the tracer concentration is observed in the larger volume of the homogenised batch. To be able to consider the difference from this point of view, it is necessary to evaluate the measured volume or the observation scale V_m . When radiotracers are used, the detection probe can be situated outside the unit. The measured space is given not only by the shielding, collimation opening and energetic properties of the tracer in the measured media, but also by the detector properties. The larger the collimation opening or closer distance of the detector from the wall of vessel, the larger is the measured volume. The radiotracer with higher radiation energy is registered by the detector from a longer distance. Each elementary part of the detected volume, however, contributes in a different way to the total radiation recorded. Therefore, it is evident that theoretical evaluation of the measured volume or observation scale is quite difficult.

The capability of detection chain was tested by point source response experiments with radiotracers (see Fig. 1c) and shielding was also tested by measurement of energy spectrum for different position of the point source.

The results of evaluation of homogenisation measured by different tracers are summarised in Table 1.

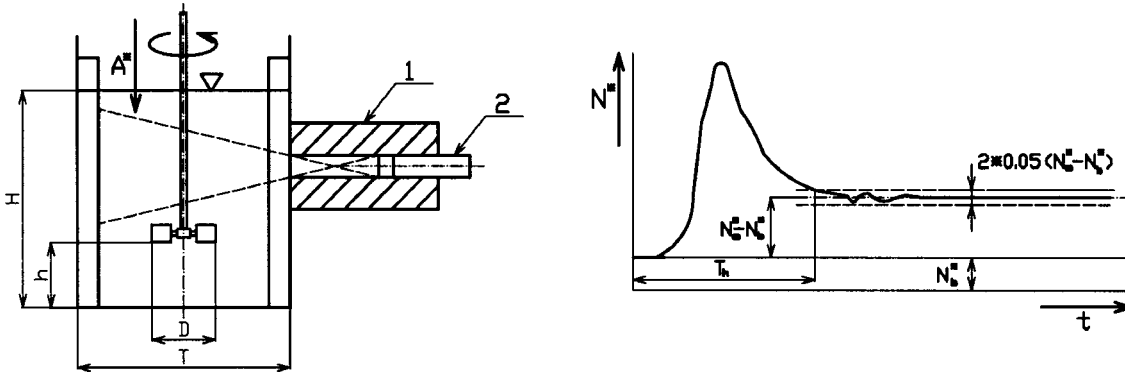


Fig. 1b. Homogenisation time evaluation; 1 – shielding; 2 – scintillation detector.

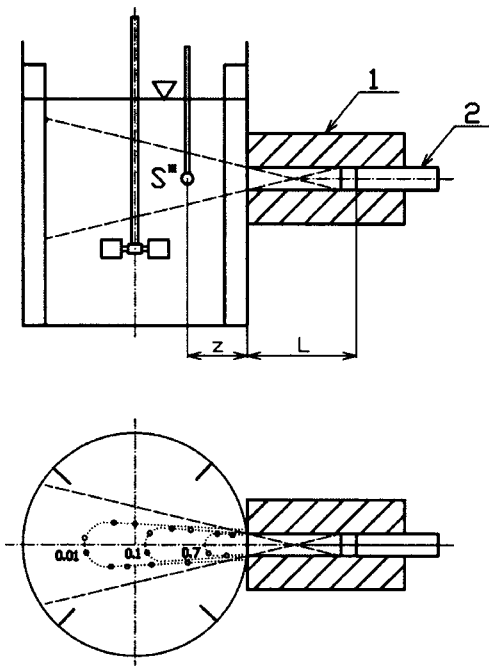


Fig. 1c. Point source response experiment.

The ratio of measured volume and total liquid volume is the scale of scrutiny $\alpha = V_m/V$. For measurement with conductivity probe, $\alpha = 10^{-4}$ (estimated measured volume by conductivity probe is $V_m = 0.64$ ml).

Simulation of homogenisation by CFD

From a numerical point of view, flows in mixing tanks are difficult to compute because of the interaction of the rotating impeller with stationary baffles on the periphery of the tank. Multiple Reference Frames (MRF) technique with multiple mesh frames is used, where one frame is attached to the rotating impeller and the other remains stationary with the tank baffles.

Velocity field evaluation (stationary simulation)

The commercial software FLUENT with a pre-processor MixSim 1.7, created by Fluent Inc. for agitated vessels, was used for the computation. All

geometry specifications of the mixing vessel and fluid properties used in the experiments were defined. The only other selected parameter was the density of the mesh. It is given by the number of the cells per the diameter of the vessel T .

A structured mesh was prepared by this software – however with a limit of 500,000 nodes in the vessel, which enabled to prepare a mesh with 3×10^5 elements. The mesh generated by the MixSim 1.7 with 3×10^5 cells is presented in Fig. 2a.

After mesh creation, specification and evaluation was done in FLUENT 6.1. Standard $k-\epsilon$ turbulence model was used for velocity field evaluation, for 5 rps, rotational speed of impeller and the results were compared with radial and axial velocity components published by different authors for a similar system [2–4, 8, 15]. From the curves A and experimental data presented in Figs. 3c and 3d, it is apparent that the results were defective especially in the region near the impeller.

In the next step, the vessel geometry was generated by MixSim 2.0 and denser unstructured mesh similar

Table 1. Time of homogenisation measured with different tracers evaluated for $\xi = 0.05$.

Re	N	Tracer	n	T_h	Var	NT_h
54,000	15	KCl	10	3.5	4.1	52.5
		^{198}Au	10	2.3	10.2	34.5
36,000	10	KCl	36	5.7	5.4	57.0
		^{198}Au	15	3.7	7.5	37.5
		^{82}Br	11	3.5	9.3	35.2
		^4Na	10	3.5	11.9	35.2
18,000	5	KCl	33	10.2	3.8	51.0
		^{198}Au	15	8.6	10.7	42.8
		^{82}Br	11	6.5	8.0	32.6
		^4Na	10	6.3	14.2	31.1
6350	5	KCl	10	9.1	4.1	36.5
		^{198}Au	9	7.3	8.7	36.5
2430	5	KCl	9	8.9	2.7	44.4
		^{198}Au	9	6.2	13.1	31.2

$Re = ND^2\rho/\mu$ – Reynolds mixing number, N [rps] – speed of stirrer revolution, n – number of experiments, T_h [s] – time of homogenisation, NT_h – dimensionless time of homogenisation, Var [%] – variation coefficient of T_h .

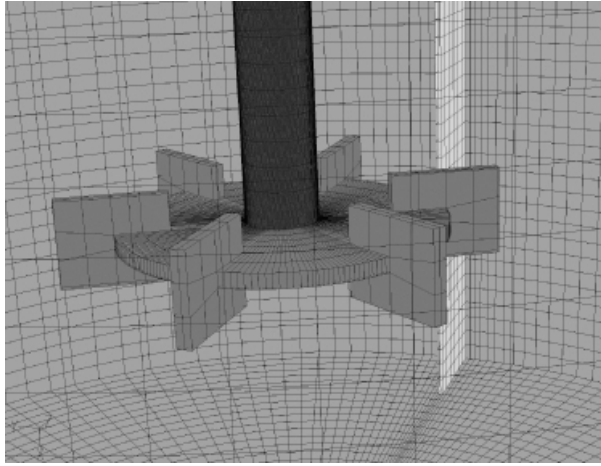


Fig. 2a. Structured mesh with 3×10^5 elements.

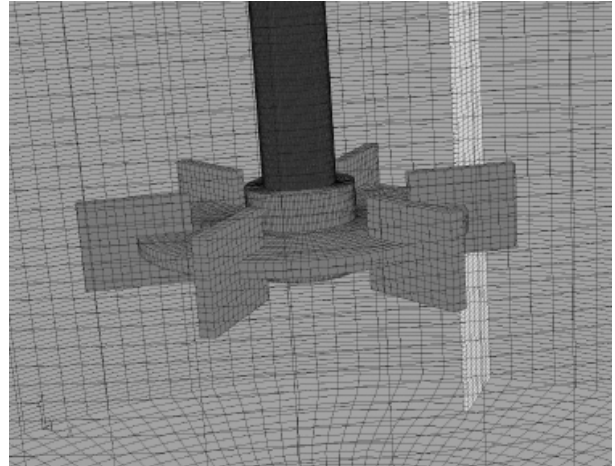


Fig. 2b. Unstructured mesh with 7×10^5 elements.

to MixSim 1.7 mesh was generated in Gambit 2.1 pre-processor (see Fig. 2b).

A new unstructured mesh was prepared with hexahedra in the whole region except the wedge cells below the shaft around the vessel axis. The dimensions of rotating frame were r (distance from the axis) = 0.058 and $0.041 < x$ (distance from the bottom) < 0.079 . More precise geometry (with a hub of the real impeller) was used in generation of the new mesh with 7×10^5 elements. Velocity fields were calculated for the structured and unstructured mesh by FLUENT 6.1, for 5 rps rotational speed of the impeller. Velocity fields in vertical and horizontal cross-section of the vessel are presented in the Figs. 3a and 3b – on the left side for structured and for unstructured mesh on the right side of the figures.

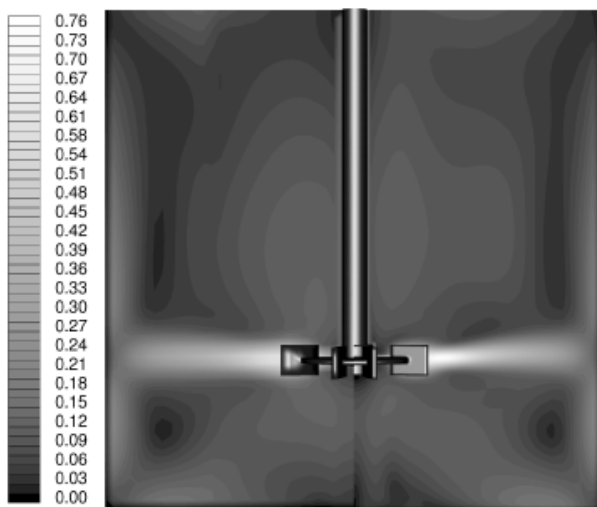
Velocity fields around the impeller on the right sides of the figures (i.e. for the more realistic mesh prepared in Gambit) present higher values of velocities, what is evident from both figures. Calculated velocities in radial and axial directions for our system (with $D = 0.3T$, $H = D$ see Fig. 1a) were compared with experimental

results of measurements by LDA (Laser Doppler Anemometry) for a similar system (with $D = T/3$), presented by several authors [2–4, 8, 15] (see Figs. 3c and 3d).

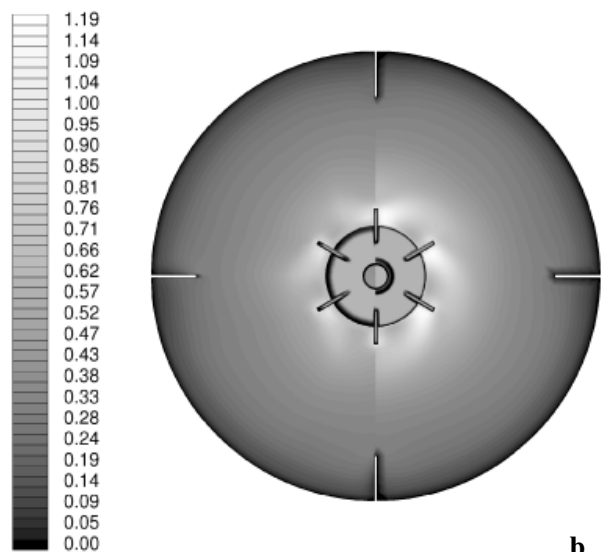
On the basis of presented comparison, the velocity field calculated by unstructured mesh was used for the next simulation of homogenisation.

Tracer distribution evaluation (unsteady simulation)

The “frozen” velocity, pressure and turbulence fields evaluated from the stationary simulation were used for unsteady solution of tracer transport equation describing tracer homogenisation. The flow inside the mixed vessel is assumed to be fully turbulent and the influence of turbulence is described by the standard k - ϵ model. This model successfully corresponds to experimental data of several authors [6, 7, 9]. The eddy viscosity concept is used for modelling the influence of turbulence as an increase in the diffusive transport (effective viscosity).



a



b

Fig. 3a, b. Contours of velocity magnitude [m/s] in vertical and horizontal cross-sections (in half between baffles), for structured on the left side and unstructured mesh on the right side.

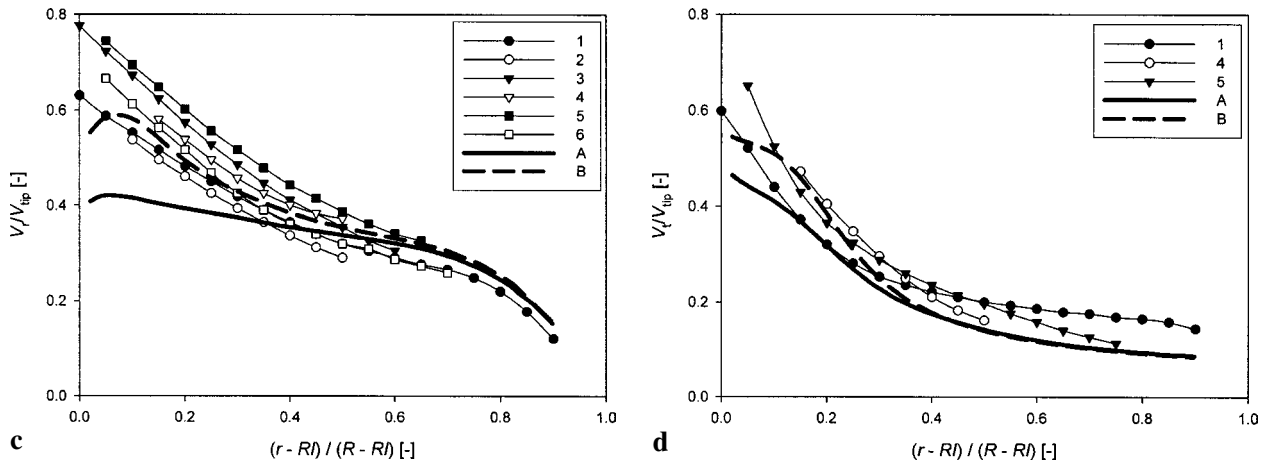


Fig. 3c,d. Comparison of calculated and measured radial and tangential component of velocity, where A-curve is calculated on structured and B-curve on unstructured mesh and experiments: 1 [2], 2 [3], 3 [15], 4 [4], 5 (H. Wu and G. K. Patterson – private communications, given in [9]), 6 [8]; $RI = D/2$ radius of stirrer; R – radius of vessel.

FLUENT computes the changes of diffusive transport by changing the value of turbulent Schmidt number [5], ($Sc = \mu/\rho D_i$, where μ , ρ is the liquid viscosity and density, while D_i is the effective mass diffusion coefficient). Tracer dispersion – homogenisation is analysed by experiment when a tracer of limited volume is added below the mixed liquid level and its dispersion in time and space is measured (tracer fluid has the same properties as the liquid filling the vessel). At the beginning of the simulation, a tracer with mass fraction 1 was added to the cluster of elements which create a sphere with a diameter of 0.01 m and this sphere is situated 0.02 m below the liquid level in the same position as in the real experiment. Tracer concentration changes in time in the whole system (with a time step of 0.01 s) were evaluated. The local tracer concentration in the probe positions could be seen and analysed.

Time of homogenisation is the time when no curve exceeds a certain range ($\xi = \pm 5\%$) around the final value.

Several numerical experiments were done. The influence of the turbulent Schmidt number presented in Fig. 4a is an example of such analysis.

Tracer dispersion – homogenisation evaluated for two positions, where different velocities (low and high)

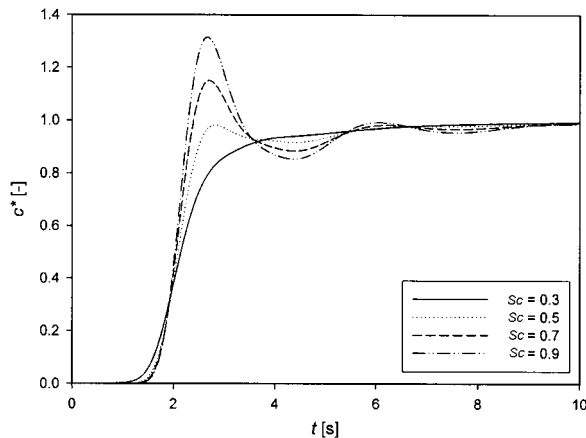


Fig. 4a. Influence of turbulent Schmidt number on homogenisation curve.

can be expected, is another example. The analysis was done for 5 rps and two different values of Sc . The changes of homogenisation caused by turbulent dispersion are evident from the Fig. 4b.

The curves for low values of turbulent dispersion ($Sc = 10$) will probably not have so many peaks and there will not be a great time delay for the curve with low velocity, in case of strong influence of numerical diffusivity. On the basis of this analysis, it may be assumed that this effect is not significant.

Simulated homogenisation curves (calculated for $0.3 < Sc < 1$ and for different positions of injection) were compared with measured results for conductivity probe. The best correspondence between the measured and simulated time of homogenisation was obtained for $Sc = 1$ and for the position of the tracer injection that was shifted towards the middle, between the rotating region and the vessel wall (little beyond the position in real experiment). The first order upwind scheme – with good results for the residual convergence – was used in the numerical simulation. Because application of this discretisation scheme may introduce a numerical error, the last evaluations were done also with quadratic

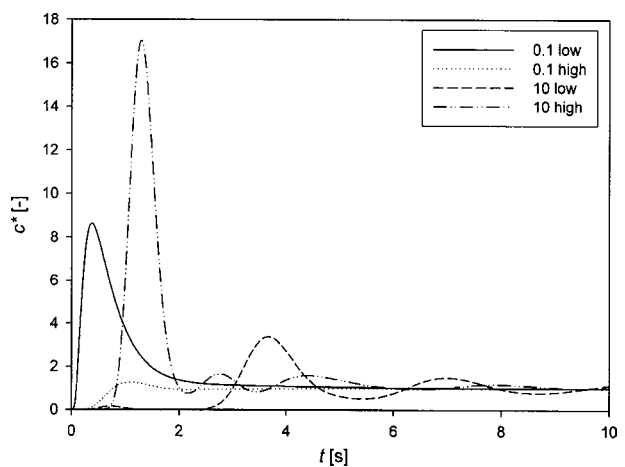


Fig. 4b. Homogenisation in two localities with different velocities for different $Sc = 0.1$ and 10, where c^* is dimensionless tracer concentration ($c^* = c(t)/c(\infty)$).

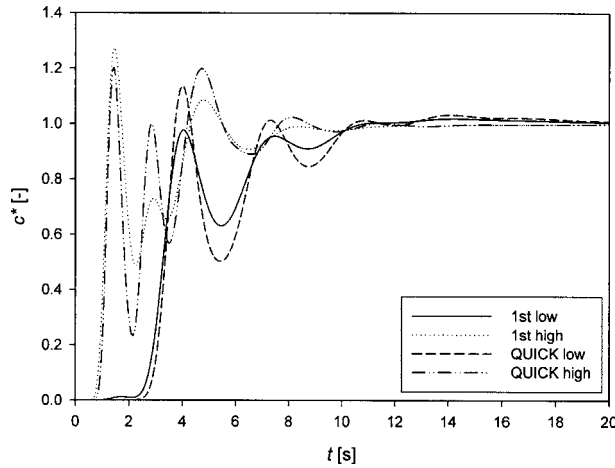


Fig. 4c. Influence of discretisation formula.

upwind interpolation scheme, which provides a higher order accuracy, however it is more time consuming.

A comparison of homogenisation curves for the discretisation scheme of the first and second order (QUICK) – for 5 rps and $Sc = 1$ – is presented in Fig. 4c.

The first order (upwind) discretisation scheme decreases fluctuation of the homogenisation curves and this tendency can change the results of time homogenisation evaluation.

Homogenisation time is evaluated from the homogenisation curves on the basis of the definition mentioned above (see also Fig. 1b). When the radiotracer is used in the homogenisation analysis and the change of tracer concentration is measured by the detector (which is situated outside of the vessel – close to the wall i.e. in position x', y', z'), registered values are given by

$$(2) \quad N(t, x', y', z') = \iiint_V D(x, y, z) c(t, x, y, z) dx dy dz,$$

where $c(t, x, y, z)$ is the distribution of tracer concentration obtained from CFD calculations, $D(x, y, z)$ is the transfer function which can be calculated, for example, by algorithms of collimated detectors, and x', y', z' describe position of the detector.

The algorithm called ‘view factor’ was suggested for narrow beam radiation and for a tracer with ‘soft’ gamma radiation [13]. The algorithm was tested on the basis of the PSR of detector in the water and is recommended for the energy of tracer about 100 keV. In the case of ^{198}Au with energy equal to 410 keV, the energy spectrum of ‘point source’ was measured in different positions in front of the detector, inside the vessel. In the case of using monoenergetic tracer with energy higher than 100 keV, it is possible to recommend – on the basis of this analysis – measurement in an ‘energetic window’. The classical isoparametric functions [16] were used for integration in the finite solution of elements.

$D(x, y, z)$ can also be received as a response of collimated detector to the ‘point’ radioactive source (PSR), which is situated inside the vessel. PSR can be created directly by experiment (if possible), or by numerical simulation by Monte Carlo code, which is implemented in program INSPECT [14]. The experiments using PSR inside the vessel (with liquid but

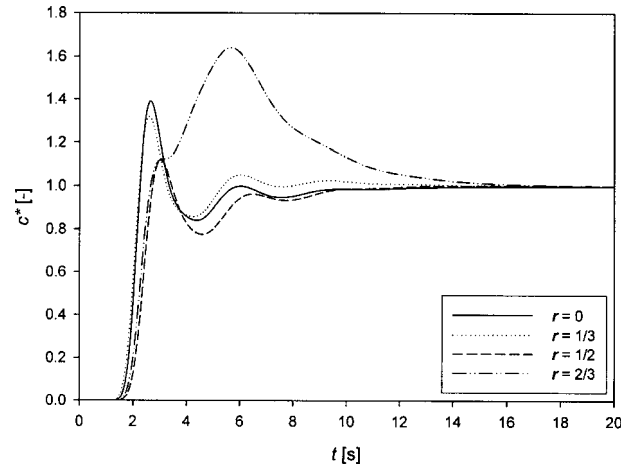


Fig. 4d. Influence of position of tracer injection on homogenisation curves, where $r = r/R$ (R is radius of the vessel).

without mixing) give information about the actual collimated detector characteristics and information about absorption and reflection characteristics of the media and internals inside the vessel. By monitoring count rate of the collimated detector at different positions of radiation source, the response function $D(x, y, z)$, corresponding to unit activity at a general point x, y, z , can be obtained (see Fig. 1c). As there are big differences between the density of measured points in PSR and density of mesh used in FLUENT evaluation, interpolation formula (presented in [13]) has to be used. Also special software has to be at disposal by which the relevant information can be extracted from the results calculated by FLUENT (which have a form of ASCII files) and which evaluates integral (2) for the position of collimated detector (for more information see [12]).

No special software is needed when only estimation of the homogenisation time measured with different radiotracers is required. It can be assumed that main contributions to the detected values are concentrations in cells which are just in front of the collimation aperture with surface F . Assuming that cells in the length step of $\Delta z/2$ represent mean tracer concentration in the volume $F\Delta z$, we can use the results of PSR measurement described by (see [11]).

$$(3a) \quad N^*/N_0^* = (L^2/(L+z)^2)k_1 \exp(-k_2 z) = D(z)$$

where constants k_1 and k_2 depend on the collimation (i.e. on diameter of the collimation aperture or surface F), on the distance of the detector from the wall of the vessel L , on the radiation energy of the used radiotracer and on the surrounding in the vessel; z is the distance of the point source from the wall of the vessel (see Fig. 1c).

The detected homogenisation curve can be finally evaluated by

$$(3b) \quad N(t, x', y', z') = F \int D(z) c(t, z) dz$$

or

$$(3c) \quad N(t, x', y', z') = F \sum_i D(z_i) c(t, z_i) \Delta z.$$

Table 2. Influence of position of tracer injection on homogenisation time [s] measured in the cell (= position of conductivity probe).

Position of tracer injection from the shaft of stirrer	Homogenisation time T_h [s]
$r/R = 0$	7.9
$r/R = 1/3$	6.16
$r/R = 1/2$	8.57
$r/R = 2/3$	12.3

Results and conclusion

From the experimental diagrams of homogenisation, it follows that the longest time of homogenisation is obtained by the conductivity probe (with small measured volume) and then with ^{198}Au , ^{82}Br and ^{24}Na . Good correspondence of simulation with the conductivity method was received after small shifting the position of injection. The influence of the position of the tracer adding on the homogenisation curves is demonstrated in Fig. 4d and the results are summarised in Table 2.

The change of homogenisation time with position of cells situated in front of the detector was evaluated for the position of tracer injection $r/R = 2/3$. The situation is shown in Fig. 5a and the results of the simulation calculated for 5 rps, $Sc = 1$, time step $dt = 0.01$, and for 2nd order of discretisation scheme are presented in Fig. 5b.

There are evidently greater values of homogenisation time for the regions close to the wall of the vessel; the shorter time of homogenisation behind the shaft of stirrer is probably the result of shorter distance from the position of tracer injection. Similar trend was obtained also for the 1st order of discretisation, but the values of homogenisation time in the case of using the 2nd order are more realistic (when QUICK scheme was used [5]).

The results of homogenisation time evaluated for different positions of cells for the 2nd order of discretisation scheme were used as the mean values for the region of 1 ml. Supposing that the volume of region is the measured volume V_m , the scale of scrutiny in the vessel of $V = 6280$ ml is $\alpha = V_m/V = 1/6280 \sim 1.6 \times 10^{-4}$.

Mean values of tracer concentration for two, three,... and 18 positions (i.e. for volume of two, three,... and 18 ml, i.e. for $\alpha = 3.2, 4.8, \dots$ and 28.6×10^{-4}) were calculated in every time step in two sequences – from the detector to the opposite vessel wall and in the reverse sequence from the wall to the detector. The time of homogenisation for given values of α could be evaluated from the homogenisation curve. The results are shown in Fig. 5c together with experimental dependence $T_h = -1.27 \ln \alpha$, obtained by the conductivity method with different volume probes in the same system [10]. This results from this simulation that the dependence of time of homogenisation on the scale of scrutiny is influenced by the position of detectors.

Finally, the results of tracer concentration in different positions in front of the detector were used for estimation of time of homogenisation measured with

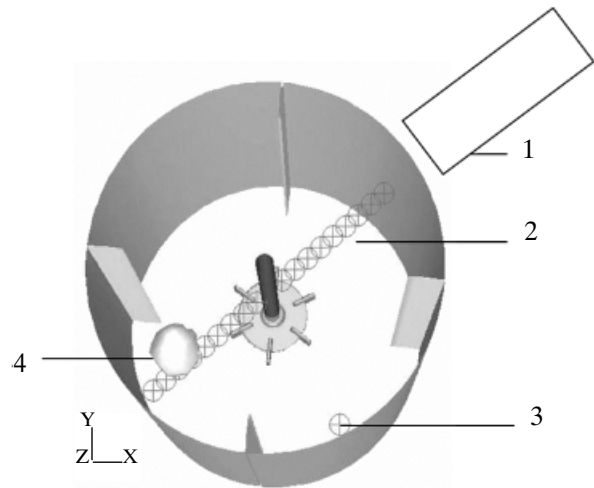


Fig. 5a. Geometrical conditions of simulated experiment: 1 – collimated detector; 2 – position of cells; 3 – position of conductivity probe; 4 – tracer injection.

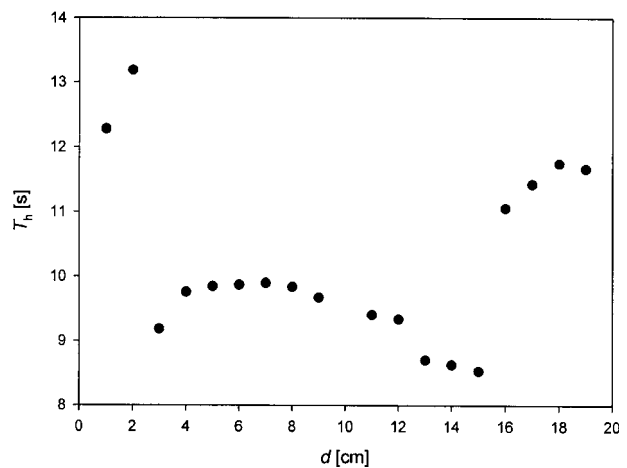


Fig. 5b. Time of homogenisation T_h in elements situated at different distance d from the detector.

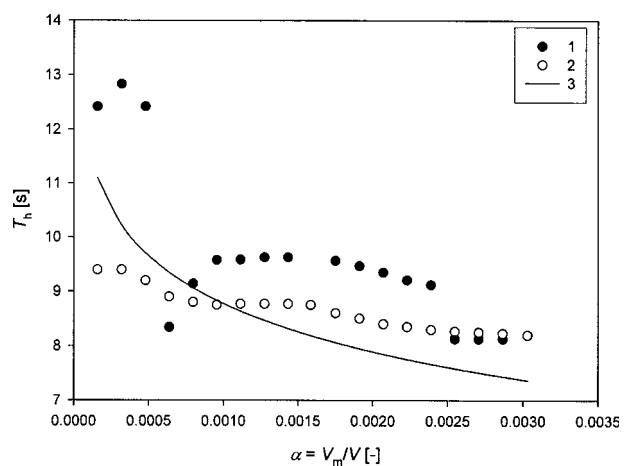


Fig. 5c. Time of homogenisation T_h as a function of scale of scrutiny α ; 1 – simulation, data from probes sequenced from the detector to the opposite vessel wall; 2 – simulation, data from probes in opposite sequence from the vessel wall to the detector; 3 – experimental dependence obtained by different method in different volume of the vessel (see [11]).

Table 3. Homogenisation time T_h [s] – measured and simulated with different tracer.

Methods	5 rps				10 rps				15 rps	
	KCl	¹⁹⁸ Au	⁸² Br	²⁴ Na	KCl	¹⁹⁸ Au	⁸² Br	²⁴ Na	KCl	¹⁹⁸ Au
Experimental confidence interval ⁾	10.3 10.0–10.6	8.6 7.9–9.3	6.5 6.0–7.0	6.5 5.3–7.3	5.7 5.6–5.9	3.7 3.5–3.9	3.5 3.2–3.8	3.5 3.0–3.9	3.6 3.4–3.7	2.3 2.0–2.6
CFD simulation	10^{**}				5				3.4	
CFD – detector algorithm		8.2				4.2				2.8
CFD-PSR estimation		8.24	7.0	6.2		4.4	3.4	3.3		3.1

⁾ Symmetrical confidence interval was evaluated for confidence coefficient = 0.99.

^{**}) Results in bold are inside of confidence interval.

different radiotracers. In this case, tracer concentration $c(t, z_i)$ in time (t) and position (z_i), were multiplied by value of the weight function $D(z_i, \text{tracer})$ received from the PSR experiment for the given position (z_i) and used radiotracer i.e. by Eqs. (3a) and (3c). This operation was done for all 18 positions in front of the detector for every time step during the homogenisation, so the homogenisation time could be evaluated easily from the homogenisation curve $C^*(t) = \sum c_i(t) D_i$. The evaluated values of homogenisation time for the used radiotracers ¹⁹⁸Au, ⁸²Br and ²⁴Na estimate the measured values very well (see Table 3).

Acceptable comparison of CFD simulation by using the ‘view factor’ with using the integral energy measurement by ¹⁹⁸Au (=0.41 MeV and linear absorption coefficient in water = 10.5 m⁻¹) was also obtained. The results are summarised in Table 3.

A method using CFD and results of PSR for the whole field of tracer concentration, which demands special post-processing of data, is prepared for testing.

Conclusions

CFD simulation of homogenisation using the standard k - ϵ turbulence model is sensitive to probe position and region of tracer injection than in the real experiments (which were done in a small vessel). Numerical diffusion does not have a strong influence on the homogenisation time simulation, however discretisation scheme of higher order is recommended. On the basis of numerical simulation, it was shown that the dependence of homogenisation time on the volume of the probe (scale of scrutiny) can be influenced by position of the probes.

CFD simulation of homogenisation time measured with a radiotracer by using the ‘view factor’ as algorithm for detection was successful for ¹⁹⁸Au (which has the lowest energy from the radiotracers used in the experiments). The estimation of homogenisation time on the basis of CFD simulation of the tracer concentration in positions in front of detector and on the basis of weight function obtained by measurement of PSR offers acceptable results for the used tracers (¹⁹⁸Au, ⁸²Br and ²⁴Na).

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