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# The computer simulation of mixing of non-Newtonian fluid in 2-D semi-cylinder cavity

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In this paper some results of the computer simulation of mixing of non-Newtonian fluid are presented. Numerical calculations were done for dimensionless form of the equations of motion for the Carreau fluid in incompressible and viscous flow in a two-dimensional semi-cylindrical cavity. The full Navier–Stokes equations for the Carreau fluid were written in velocity–vorticity, and next in finite difference form. The solutions were accomplished by finite time-step advancement. The mixing process was studied by tracking the motion of particles in the mixing region. The particles were represented by marked points. The mixing efficiency was quantified in terms of the average distance between the tracer particles and the centroid of the particle distribution.

**Keywords:** Carreau fluid, FDM, mixing process

## 1. Introduction

Non-Newtonian fluids have many applications in modern industry. Applications of non-Newtonian fluids, e.g. polymer processing, require understanding of the processes, which occur during the fluid mixing. Among non-Newtonian fluids oil, mixture of oil with water (emulsion) and human blood are most notable. The current practice of designing industrial mixers for fluids with complicated rheological model (e.g. Carreau model) should be supported by science. However, non-Newtonian nature of fluid is not understood well enough. Complicated geometry of mixers and fluid rheology (Jurkowski and Jurkowska [6]) still remain the subject of scientific research and topic of articles. Polymer blends can be obtained, for example, during dispersive mixing in the dynamic mixer (shear head). Few examples of mixers are presented by Jurkowski and Jurkowska [6]. Hindmarch [5] presents the Cavity Transfer Mixer, which is a dynamic mixer. Semi-cylindrical cavity is a basic part of the Cavity Transfer Mixer.

With the framework of Newtonian fluid dynamics, the flow driven in a cavity is a widely accepted benchmark problem consisting of a bulk flow flowing past a cavity in which the fluid moves due to shear exerted by the bulk of flow. Thus, the flow in a cavity has been the subject of research of many authors. For example, Vynnycky and Kimura [10] presented a complete numerical computation of the Navier–Stokes equations for the Newtonian steady flow within a two-dimensional quarter-cavity. High accuracy approximations to the solution of N–S equations were obtained for the model problem of a driven cavity (Gupta [4]). On the other hand, one can find only few papers related with investigation on non-Newtonian flow in a cavity.

The purpose of the present paper is investigation of the mixing process during two-dimensional time-dependent, incompressible flow of non-Newtonian fluid in a semi-cylindrical cavity. Upper wall of cavity is moving at a velocity described by function:

$$\begin{aligned} u^*(t) &= u_0 \sin\left(\frac{2\pi t}{P}\right) \qquad \text{for } t \in \langle jP\,,\ (j+\tfrac{1}{2})P\rangle, \\ u^*(t) &= 0 \qquad\qquad\qquad\quad \text{for } t \in \langle (j+\tfrac{1}{2})P\,,\ (j+1)P\rangle, \end{aligned} \tag{1}$$

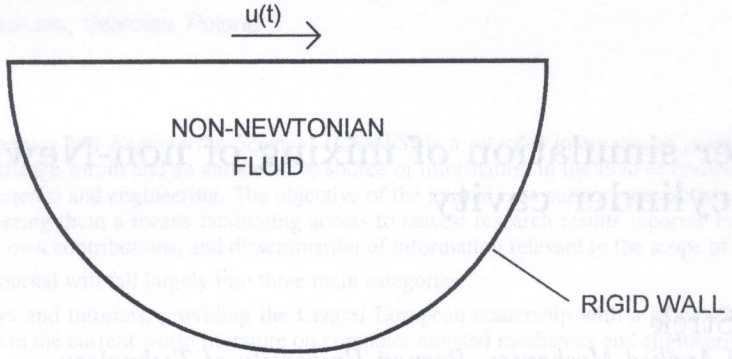


**Fig. 1.** Semi-cylindrical cavity

where $u_0$ is characteristic velocity, $j \geq 0$ and $P$ is real number. The diameter of cavity is equal to $l_0$ (characteristic length).

Numerical calculations are considered for the Carreau model of non-Newtonian fluid. The mixing process is studied by tracking the motion of particles in the mixing region.

## 2. Equation of motion for Carreau fluid

### 2.1. Basic equations

The basic model for the fluid dynamics representing two-dimensional flow of an incompressible viscous fluid is given by the Navier–Stokes equations that represent the conservation of mass and momentum. These equations are highly non-linear and are very difficult to solve.

The continuity equation (the conservation of mass) for incompressible fluid (Gryboś [3]) is:

$$\nabla \cdot \mathbf{v}^* = \mathbf{0} \tag{2}$$

where $\mathbf{v}^*$ is velocity.

Before deriving the conservation of momentum equation, let us define the stress tensor fluid:

$$\mathbf{T}^* = -p^*\mathbf{I} + \mathbf{S}^* \tag{3}$$

where

$$\mathbf{S}^* = \eta^*(\gamma)\,\mathbf{G}^* \tag{4}$$

and $\mathbf{S}^*$ is extra stress tensor, $\mathbf{G}^* = \nabla\mathbf{v}^* + (\nabla\mathbf{v}^*)^{\mathrm{T}}$ – rate of strain tensor, $\mathbf{I}$ – unit tensor, $p^*$ – pressure.

Principal form of the equation of motion of a fluid (conservation of momentum) is represented by the following Navier–Stokes equation:

$$\rho\left(\frac{\partial \mathbf{v}^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla\mathbf{v}^*\right) + \nabla p^* - \nabla \cdot \mathbf{S}^* = \mathbf{0}\,. \tag{5}$$

The rheological model of the fluid used in this study is the Carreau model (Niederkorn and Ottino [7]):

$$\eta^*(\gamma) = \mu_0\left(1 + (\lambda_c\gamma)^2\right)^{\frac{N-1}{2}}, \tag{6}$$

where we define $\gamma = \sqrt{\frac{1}{2}II}$, and $II$ is the second invariant of the rate of strain tensor, $N$ is the shear index, $\mu_0$ is the characteristic viscosity and $\lambda_c$ is time constant.

This model has several advantages over the power-law equation, $\eta^*(\gamma) = \mu_0\gamma^{N-1}$. Power-law fluids are widely used for many industrial problems. Carreau fluid does possess a characteristic viscosity and can be made dimensionless. If $N = 1$ or $\lambda_c = 0$, we have Newtonian fluid. Many polymer solutions and melts were successfully described by means of this model.

### 2.2. Dimensionless form of the equations

Let us apply the adequate characteristic scale parameter to the two-dimensional governing equations to obtain their dimensionless form. To this end, the following dimensionless groups are used:

$$\mathbf{v} = \frac{1}{u_0}\mathbf{v}^*, \qquad \mathbf{x} = \frac{1}{l_0}\mathbf{x}^*, \qquad t = \frac{t^*}{t_0}, \qquad \eta(\gamma) = \frac{1}{\mu_0}\eta^*(\gamma)\,.$$

The superscribed upper-index represents the dimensional variables. In consideration of a 2-D flow we have $\mathbf{v} = [u, v]$ and $\mathbf{x} = [x, y]$.

The dimensionless form of the equations of motion for the Carreau fluid is:

$$Re\left(Sr\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) + \nabla p - \nabla\cdot\mathbf{S} = \mathbf{0} \tag{7}$$

where

$$\mathbf{S} = \left(1 + (Cr\gamma)^2\right)^{\frac{n-1}{2}}\mathbf{G}\,, \tag{8a}$$

$$\mathbf{G} = \nabla\mathbf{v} + (\nabla\mathbf{v})^{\mathrm{T}}\,, \tag{8b}$$

and $Re$ is the Reynolds number – we define it as $Re = \frac{l_0\rho u_0}{\mu_0}$, $Sr$ – Strouhal number – $Sr = \frac{l_0}{u_0 t_0}$, $Cr$ – Carreau number – $Cr = \lambda_c\frac{u_0}{l_0}$.

Two dimensionless numbers characterise the non-Newtonian nature of the flow: the shear index ($N$) and the Carreau number ($Cr$). The Carreau number can be regarded as a dimensionless shear rate.

### 2.3. Stream and vorticity functions formulation

The equation of continuity allows to introduce the stream function $\psi$ in terms of which

$$u = \frac{\partial\psi}{\partial y}\,, \qquad v = -\frac{\partial\psi}{\partial x}\,, \tag{9}$$

and vorticity

$$\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\,. \tag{10}$$

The derivation of Eqs. (7) with respect to $x$ and $y$, and elimination of $p$ gives the governing equation of two dimensionless equations of motion of an incompressible fluid in terms of stream and vorticity functions. After some mathematical manipulations we can write Eqs. (2) and (7) as the following equations:

$$\nabla^2\psi = \omega\,, \tag{11}$$

$$Re\left(Sr\frac{\partial\omega}{\partial t} + \mathbf{v}\cdot\nabla\omega\right) = \eta(\gamma)\nabla^2\omega + NN \tag{12}$$

where

$$NN = \frac{\partial\eta}{\partial y}\left(2\frac{\partial^3\psi}{\partial y^3} + \frac{\partial^3\psi}{\partial x^3} - \frac{\partial^3\psi}{\partial x\partial y^2}\right) - \frac{\partial\eta}{\partial x}\left(2\frac{\partial^3\psi}{\partial x^2\partial y} - \frac{\partial^3\psi}{\partial x^3} + \frac{\partial^3\psi}{\partial x\partial y^2}\right)$$
$$+ 2\frac{\partial^2\psi}{\partial x\partial y}\left(\frac{\partial^2\eta}{\partial x\partial y} + \frac{\partial^2\eta}{\partial x^2}\right) - \frac{\partial^2\psi}{\partial x^2}\left(\frac{\partial^2\eta}{\partial y^2} - \frac{\partial^2\eta}{\partial x\partial y}\right). \tag{12a}$$

Using the stream function we can write scalar measure of the rate of strain tensor as:

$$\gamma = \sqrt{4\left(\frac{\partial^2\psi}{\partial x\partial y}\right)^2 + \left(\frac{\partial^2\psi}{\partial y^2} - \frac{\partial^2\psi}{\partial x^2}\right)^2}\,. \tag{13}$$

### 2.4. Boundary and initial conditions

In consideration of 2-D flow in a cavity we have $\mathbf{v} = [u, v]$ and the following boundary conditions: $\mathbf{v} = [0, 0]$ for fixed part of cavity and $\mathbf{v} = [u(t), 0]$ for moving one. As an initial condition we assume $\mathbf{v} = [0, 0]$ for the whole cavity.

The boundary conditions on the stream function are:

- $\psi = 0$ and $\partial\psi/\partial\bar{n}$, for the non-slip part of the cavity where $\bar{n}$ is the vector normal to the boundary,
- $\psi = 0$ and $\partial\psi/\partial y = u(t)$, for the moving wall of the cavity.

Upper wall is moving at velocity $u(t) = \frac{1}{u_0}u^*(t)$.

## 3. Description of the method

### 3.1. Method of solution

Observe that Eqs. (11)–(12) is a coupled system of non-linear partial differential equations in $\psi$ and $\omega$. But when $\omega$ is known, then Eq. (11) is a linear elliptic equation in $\psi$, while if $\psi$ is known, then Eq. (12) is a linear parabolic equation in $\omega$. This suggests making initial guesses $\psi_n^0$ and $\omega_n^0$ for $t = t_n$ from the initial conditions or the previous time cycle. Now we can use $\omega_n^0$ in Eq. (11) to derive $\psi_n^1$. Next we use $\psi_n^1$ in Eq. (12) to derive $\omega_n^1$. In general, we can use $\omega_n^i$ in Eq. (11) to derive $\psi_n^{i+1}$ and use $\psi_n^{i+1}$ in Eq. (12) to derive $\omega_n^{i+1}$. If the sequences $\omega_n^i$ and $\psi_n^i$ converge, when $\max(|\psi_n^i - \psi_n^{i-1}|, |\omega_n^i - \omega_n^{i-1}|) < \varepsilon$, where $\varepsilon$ is a small real number – we might hope that they would converge to the solution $\omega_n$ and $\psi_n$ of the given problem for $t = t_n$. We can apply mentioned algorithm for all $t_n$, so we obtain the values of stream and vorticity functions.

### 3.2. Finite difference method

The algorithm used in this study is based on the Finite Difference Method (Greenspan [2] and Roache [8]). In order to apply this algorithm, we have to approximate equations (11)–(12) by the finite difference equations. Greenspan proposed the above algorithm for the equations of motion for Newtonian fluid. The Newtonian flow is obtained by setting $NN = 0$ in (12). The dropped part of equation is more complicated than the rest. Using difference formula to discretized derivatives of expression (12a) we complete Eq. (12).

If $\omega$ is known, the elliptic partial differential equation (11) we consider is the Poisson equation. The method to be used to find the values of $\psi$ in the considered region is an adaptation of the FDM for boundary-value problems.

The cavity region is divided and covered by a grid of uniform rectangular mesh ($h \times k$). The boundary is approximated by a curve coinciding with lines of rectangular mesh of the grid. This method is very popular in structural mechanics. Figure 2 presents the grid lines and mesh points of semi-cylindrical cavity. There are three kinds of mesh points: boundary mesh points, 1st interior mesh points and 2nd interior mesh points.

Let $(x, y)$, $(x+h, y)$, $(x, y+k)$, $(x-h, y)$, $(x, y-k)$, $(x+2h, y)$, $(x, y+2k)$, $(x-2h, y)$, $(x, y-2k)$ be numbered 0, 1, 2, 3, 4, 5, 6, 7, 8, respectively. For each 2nd interior mesh point of the grid for $t = t_n$ we can approximate Eq. (11) by

$$-2(k^{-2} + h^{-2})\psi_{n,0} + h^{-2}(\psi_{n,1} + \psi_{n,3}) + k^{-2}(\psi_{n,2} + \psi_{n,4}) = -\omega_{n,0}\,. \tag{14}$$

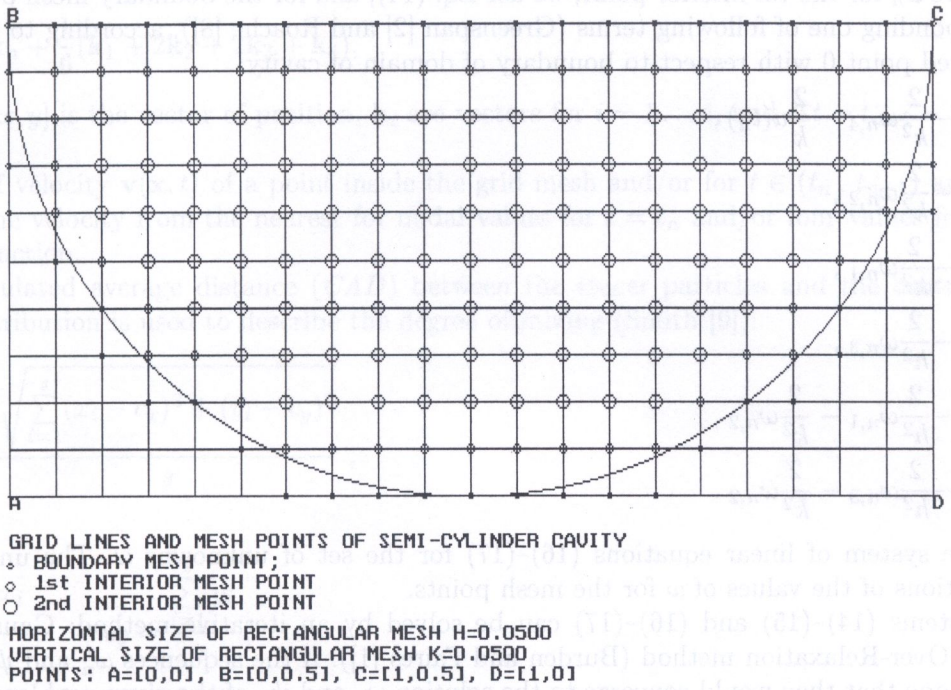


**Fig. 2.** Grid lines and mesh points of semi-cylindrical cavity

If we use information following from the boundary conditions of the problem, we can approximate Eq. (11) for the 1st interior mesh points by one of the following terms (Greenspan [2] and Roache [8]):

$$\begin{aligned}
\psi_{n,1} &= \frac{1}{4}\psi_{n,5}\,, \\
\psi_{n,3} &= \frac{1}{4}\psi_{n,7}\,, \\
\psi_{n,4} &= \frac{1}{4}\psi_{n,8}\,, \\
\psi_{n,2} &= \frac{1}{4}\psi_{n,6} + \frac{h}{2}u(t_n)\,.
\end{aligned} \tag{15}$$

We get the system of linear equations (14)–(15) for the set of unknowns $\psi$. The unknowns are approximations of the values of for the interior mesh points.

To derive $\omega_n$ from Eq. (12) we assume that $\alpha = \psi_{n,1} - \psi_{n,3}$ and $\beta = \psi_{n,2} - \psi_{n,4}$. If $\alpha > 0$ then let $A = \omega_{n,2} - \omega_{n,0}$, or else let $A = \omega_{n,0} - \omega_{n,4}$. If $\beta > 0$ then let $B = \omega_{n,0} - \omega_{n,3}$, or else let $B = \omega_{n,1} - \omega_{n,0}$.

For all 2nd interior mesh points we can approximate Eq. (12) by

$$\begin{aligned}
&\frac{Re\,Sr\,hk}{\Delta t}\omega_{n-1,0} + \left[-2\eta_{n,0}\left(\frac{h}{k}+\frac{k}{h}\right) - \frac{Re\,Sr\,hk}{\Delta t}\right]\omega_{n,0} \\
&\quad + \frac{k}{h}\eta_{n,0}(\omega_{n,1}+\omega_{n,3}) + \frac{h}{k}\eta_{n,0}(\omega_{n,2}+\omega_{n,4}) + \frac{Re\,\alpha}{2}A - \frac{Re\,\beta}{2}B + hk\,NN_{n,0} = 0,
\end{aligned} \tag{16}$$

where $\eta_{n,0}$, $NN_{n,0}$ are the values of $\eta(\gamma)$, $NN$ for $t = t_n$ at the point numbered by 0.

To derive $\omega_n$ for the 1st interior point, we use Eq. (14), and for the boundary mesh points we use the corresponding one of following terms (Greenspan [2] and Roache [8]), according to the position of considered point 0 with respect to boundary of domain of cavity:

$$\begin{aligned}
\omega_{n,0} &= -\frac{2}{k^2}\omega_{n,4} - \frac{2}{k}u(t_n)\,,\\
\omega_{n,0} &= -\frac{2}{k^2}\omega_{n,2}\,,\\
\omega_{n,0} &= -\frac{2}{h^2}\omega_{n,1}\,,\\
\omega_{n,0} &= -\frac{2}{h^2}\omega_{n,3}\,,\\
\omega_{n,0} &= -\frac{2}{h^2}\omega_{n,1} - \frac{2}{k^2}\omega_{n,2}\,,\\
\omega_{n,0} &= -\frac{2}{h^2}\omega_{n,3} - \frac{2}{k^2}\omega_{n,2}\,.
\end{aligned} \tag{17}$$

We get the system of linear equations (16)–(17) for the set of unknowns $\omega$. The unknowns are approximations of the values of $\omega$ for the mesh points.

The systems (14)–(15) and (16)–(17) can be solved by an iterative method: Gauss Seidel or Successive Over-Relaxation method (Burden and Faires [1]). If the sequences $\omega_n^i$ and $\psi_n^i$ converge, we might hope that they would converge to the solution $\omega_n$ and $\psi_n$ of the given problem for $t = t_n$. First few iterations for each time step are made for the Newtonian fluid (when $NN = 0$ for each mesh point).

Using Eq. (9) we can find the velocity vector for each interior mesh point:

$$u_{n,0} = \frac{\psi_{n,2} - \psi_{n,4}}{2k}\,, \qquad v_{n,0} = \frac{\psi_{n,3} - \psi_{n,1}}{2h}\,. \tag{18}$$

Values of the velocity vector for the boundary mesh points are known from the boundary conditions.

The flow is considered to be convergent when

$$\max\left(\left|\frac{u_{n-1,0} - u_{n,0}}{c + u_{n,0}}\right|, \left|\frac{v_{n-1,0} - v_{n,0}}{c + v_{n,0}}\right|\right) < \frac{c}{10}$$

where $c = 0.001$ from time $t_{n-1}$ to $t_n$.

### 3.3. Motion of particles in the mixing process

We study the mixing process by tracking the motion of particles in the mixing cavity. The particles are represented as massless points. The locations of the particles can be found by integrating the velocity vector with respect to time:

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{v}(\mathbf{x}, t) \qquad \text{with initial condition} \quad \mathbf{x}_0 = \mathbf{x}0 \tag{19}$$

where $\mathbf{x}0$ is the vector of position for $t = t_0$, using the Runge–Kutta fourth-order method (Burden and Faires [1]). The classical Runge–Kutta method of order four is used:

$$\begin{aligned}
\mathbf{k}_1 &= \Delta t\, \mathbf{v}(t_n\,,\, \mathbf{x}_n),\\
\mathbf{k}_2 &= \Delta t\, \mathbf{v}\left(t_n + \frac{\Delta t}{2}\,,\, \mathbf{x}_n + \frac{1}{2}\mathbf{k}_1\right),\\
\mathbf{k}_3 &= \Delta t\, \mathbf{v}\left(t_n + \frac{\Delta t}{2}\,,\, \mathbf{x}_n + \frac{1}{2}\mathbf{k}_2\right),\\
\mathbf{k}_4 &= \Delta t\, \mathbf{v}(t_{n+1}\,,\, \mathbf{x}_n + \mathbf{k}_3),
\end{aligned}$$

and

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \frac{1}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4),$$

where $\mathbf{x} = [x, y]$ is the vector of position, $\mathbf{k}_i$ are vectors for $i = 1 \ldots 4$, and $\Delta t = t_{n+1} - t_n$ for each $n \geq 0$.

Values of velocity $\mathbf{v}(\mathbf{x}, t)$ of a point inside the grid mesh and/or for $t \in (t_n\,,\, t_{n+1})$ are approximated by the velocity from the nearest for nodal values for $t = t_n$ and/or four values for $t = t_{n+1}$ by linear function.

The calculated average distance ($CAD$) between the tracer particles and the centroid of the particle distribution is used to describe the degree of mixing (Smith [9]):

$$CAD = \frac{\sqrt{\sum_{i=1}^{s}(x_i - c_x)^2 + (y_i - c_y)^2}}{s}, \tag{20}$$

where

$$c_x = \frac{\sum_{i=1}^{s} x_i}{s}, \qquad c_y = \frac{\sum_{i=1}^{s} y_i}{s},$$

and $s$ is the number of particles, $x_i$ , $y_i$ are co-ordinates of the $i$-th particle.

## 4. Simulation results

The two important flow parameters for the Carreau fluid are the Carreau number ($Cr$) and the shear index ($N$). Computer solutions were generated to study the influence of this parameters on the mixing process. We compared the values of the calculated average distance for three different fluids after a fixed time for each example of fluid.

For simplicity, we denoted by fluid A the Carreau fluid with the following parameters $Cr = 2$, $N = 0.2$; fluid B – $Cr = 2$, $N = 0.5$, and fluid C – $Cr = 5$, $N = 0.5$. For each fluid $Re = 1$ and $Sr = 1$. Carreau number is identical for fluid A and B, shear index is identical for fluid B and C.

In all examples in this paper the upper wall of cavity is moving from left to right at a dimensionless velocity $u(t)$ with $P = 0.016$, $\Delta t = 0.001$, $h = k = 0.05$.

The first particle tracking algorithm was used to study the dynamics of mixing of the fluid. The particles were represented by marked and massless points. Figures 3a–e show the effect of mixing for fluid B at various times after initiation of the flow. At time zero, 4902 particles were placed in a droplet with centre below the upper wall, as it is shown in Fig. 3a. In this case the initial calculated average distance was 0.00101.

Effect of the Carreau number and shear index on the calculated average distance and mixing process is presented in Table 1. Although in general we observe that values of $CAD$ increase as

**Table 1.** Values of $CAD$ in function of time

| Time of mixing | Fluid A $Cr = 2$, $N = 0.2$ | Fluid B $Cr = 2$, $N = 0.5$ | Fluid C $Cr = 5$, $N = 0.5$ |
|---|---|---|---|
| 0 | 0.001010 | 0.001010 | 0.001010 |
| 1 | 0.003920 | 0.001299 | 0.001104 |
| 2 | 0.004925 | 0.002242 | 0.002576 |
| 3 | 0.006368 | 0.002493 | 0.002261 |
| 4 | 0.006401 | 0.002260 | 0.004205 |
| 5 | 0.006153 | 0.003430 | 0.006521 |

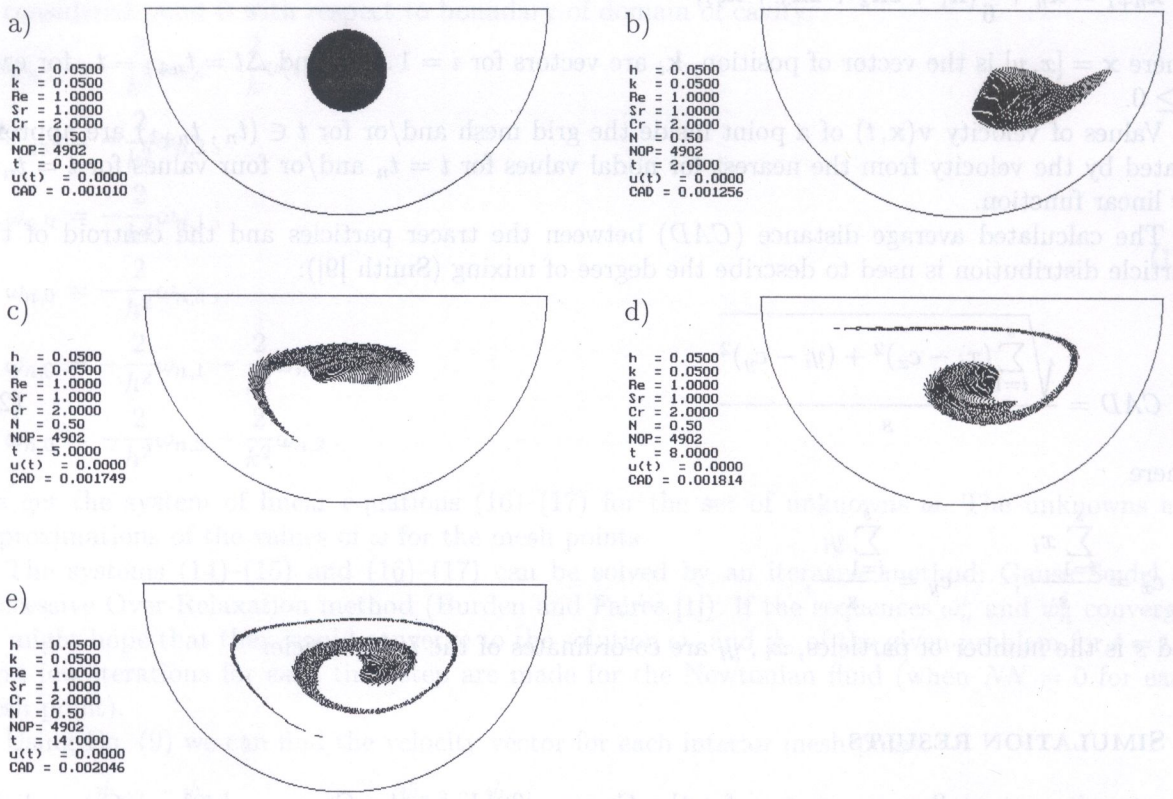


**Fig. 3.** Results of mixing for fluid A for $t = 0, 2, 5, 8, 14$

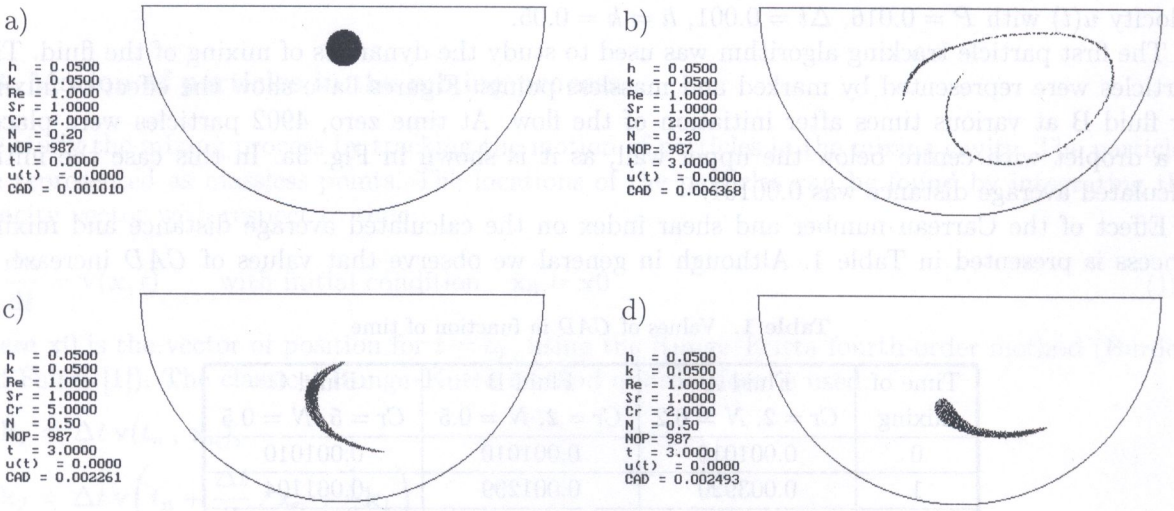


**Fig. 4.** Results of mixing for fluids A, B and C for $t = 3$

a function of mixing time, we have to notice that there are short periods of time when the value of $CAD$ decreases.

Figures 4b–c show the influence of shear index ($N$) on the degree of mixing. Figures 4c–d show the influence of Carreau number ($Cr$) on the degree of mixing. All results of mixing presented in Fig. 4 are shown for $t = 3$. At time zero, 987 particles were placed in the droplet with centre in the point shown in Fig. 4a.

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