**Femlab 3.0: Experiences in Determining RTD**

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**Introduction**

The use of commercially available Computational Fluid Dynamics (CFD) packages to study the residence time distribution (RTD) in wastewater treatment plants was recently discussed (Madeira, et. al., 2004). In that study the Fluent package (ver 6.0) ([http://www.fluent.com](http://www.fluent.com)) was used to simulate a 2-D reservoir with dimensions \( L \) (length) and \( H \) (height) in laminar flow and isothermal conditions (see Figure 1).

![Figure 1 Sketch of Reservoir Geometry](From Madeira et. al., 2004 with permission)

Both the inlet and the outlet boundaries of the reservoir have a height of 0.01 m with distances from the bottom of the reservoir of 0 an 0.02 m, respectively. Both \( L \) and \( H = 0.1 \) m.

A fully developed parabolic velocity profile is imposed on the inlet boundary

\[
u_x = U_{\text{max}} \left[ 1 - \left(\frac{y-H/20}{H/20}\right)^2 \right]
\]  

(1)

where

\[U_{\text{max}} = 1.5 \ U_{\text{mean}}\]
There is no slip at the walls ($u_x = u_y = 0$).

A step input of a component with properties similar to water ($\eta = 0.001 \text{ kg/(m-s)}$, $\rho = 1000 \text{ kg/m}^3$, with $D = 5\times10^{-10} \text{ m}^2/\text{s}$) and having constant concentration (1000 kg/m$^3$) across the inlet boundary is introduced at time zero.

**Results of the Study with Fluent**

Figures 2 and 3 indicate the results of the studies by Madeira et. al., 2004 at various Reynolds numbers with $L/H = 1$. They present a table showing the influence of Reynolds number on the mean residence time.

![Figure 2](image.png)

Figure 2. Steady state contours of the stream function for the reservoir with $L/H = 1$ as a function of Reynolds number

(From Madeira et. al., 2004 with permission)
It is the purpose of this study to see how the same problem is solved using Femlab 3.0 (http://www.comsol.com). The study is limited to Re= 10 and L/H = 1.

**Setting up Femlab**

The general procedure followed using Femlab is:

1. Solve the ns (Navier-Stokes) equation at steady state
2. Solve the cd (Convection-Diffusion) equation starting at time zero to time 500 sec in time increments of 2 sec holding constant the steady state solution of the ns equation.
3. Record the integrated exit boundary concentration at the specified times on a spreadsheet for analysis of the RTD and mean residence time.

In Femlab Enter:

*New, 2D*

*Chemical Engineering Module*

*Momentum Balance*

*Incompressible Navier-Stokes*

*Steady State Analysis* (highlighted)

Click *Multiphysics* then *Add*

*Mass Balance*

*Convection and Diffusion*

*Transient Analysis* (highlighted)

Click *Add*

Click *OK*
**Setting Up the Geometry**

In Femlab enter with respect to Figure 1 (H = 0.1, L = 0.1):

*Draw*

- *Specify Objects*
  - *Line*
    - Enter the line coordinates for each boundary of the geometry
    - Click on *Zoom Extents* (on the menu) after each line is entered.
- *Coerce to Solid*

The inlet flow boundary is assigned as boundary 1, the outlet boundary is assigned as boundary 6, the top left boundary as 3, the top boundary as 4, the top right boundary as 7, the bottom right boundary as 5 and the bottom boundary as 2.

**Setting up the Constants**

In Femlab enter:

*Options*

- *Constants*

![Femlab Constants window](image)

Figure 4. Femlab Constants window

Note (Figure 4) that \( \eta = \eta \), \( \text{den} = \rho \), \( \text{Difus} = D \) (the diffusivity) and \( \text{Co} \) is the concentration (kg/m\(^3\)) of the component at the inlet. \( \tau \) is the space-time and \( U_{\text{max}} \) is calculated from the Reynolds number as shown.
Solving the Navier-Stokes Equations

In Femlab enter (Multiphysics –ns):

Options

Expressions

Boundary Expressions
  Boundary Expression 1

  Name   Expression
  
  uvel   Umax * [1 – ((y-HH)/HH)^2]

Physics
  Subdomain Settings 1
  Physics Tab

  \( \rho = \text{den} \) Density
  \( \eta = \text{eta} \) Dynamic Viscosity

Boundary Settings

  Boundary Setting 1
  Boundary Condition  Inflow/Outflow Velocity
  \( u_0 = \text{uvel} \) x velocity
  \( v_0 = 0 \) y velocity

  Boundary Setting 2
  Boundary Condition  No Slip

  Boundary Setting 3
  Boundary Condition  No Slip

  Boundary Setting 4
  Boundary Condition  No Slip

  Boundary Setting 5
  Boundary Condition  No Slip

  Boundary Setting 6
  Boundary Condition  OutFlow/ Pressure

  Boundary Setting 7
  Boundary Condition  No Slip

Mesh
  Initial Mesh
  Refine Mesh
  Refine Mesh

(A finer mesh size was tried but memory was found to be inadequate (512 MB)).
Solve
Solver Parameters
Stationary Nonlinear
Solver Manager
Initial Value Tab
Initial Value
Check Initial Value Expressions
Fixed Solution/Linearization Initialization Point
Check Initial Value
Solve for Tab
Geom 2D
Incompressible Navier-Stokes (highlight)
Output Tab
Geom 2D
Incompressible Navier-Stokes (highlight)
Solve Problem

Postprocessing
Plot Parameters
General Tab
Check Streamline
Streamline Tab
Check Number of Start Points (60)
Click OK

Figure 5  Streamlines of the solution at Re = 10

This output compares well to the Fluent results of Figure 2 at Re = 10.
Solving the Convection-Diffusion Equation

The solution to the time dependent convection-diffusion equation (cd) proved to require considerable trial and error since the problem is so convection dominant (Comsol_a, 2004). Femlab provides a number of artificial stabilization methods (Comsol_b, 2004) which modifies the original problem. Some of the methods, however, do not provide what were judged to be reasonable solutions.

When no stabilization is used, Figure 6 is the concentration profile that occurs after 222 sec. and Figure 7 is the results after 398 sec. A negative value for the integrated concentration at the exit at 222 sec is returned and the profile at 398 sec does not seem reasonable.

Figure 6. Exit concentration profile at 222 sec with no stabilization
Both streamline diffusion and crosswind diffusion stabilization methods were tried but rejected. Isotropic diffusion was most extensively tested and was finally accepted. The tuning parameter was slowly decreased from a value of 0.5 to 0.008, the point at which the concentration profiles were still acceptable (Figures 8 and 9).
Figure 8 Exit concentration profile at 222 sec with isotropic stabilization = 0.008

Figure 9 Exit Concentration Profile at 398 sec with isotropic stabilization = 0.008
The procedure with isotropic stabilization to solve the cd equation (storing the steady state ns solution):

Enter Femlab:

**Multiphysics**
- **Convection and Diffusion (highlighted)**

**Physics**
- **Boundary Settings**
  - Boundary Selection 1: Concentration
    - Co = Co
  - Boundary Selection 2: Insulation/Symmetry
  - Boundary Selection 3: Insulation/Symmetry
  - Boundary Selection 4: Insulation/Symmetry
  - Boundary Selection 5: Insulation/Symmetry
  - Boundary Selection 6: Convective Flux
  - Boundary Selection 7: Insulation Symmetry

**Subdomain Settings**

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</table>

**Artificial Diffusion**
- isotropic diffusion $\delta_{id} = 0.008$ Tuning Parameter

**Init Tab**
- $c(t_0) = 0$ Concentration $c$

**Solve**

**Solver Parameters**
- **General Tab**
  - Solver – Time Dependent
  - Time Stepping – Time 0:2:500

**Time Stepping Tab**
- Time step taken by Solver – Strict

Some differences were noted in how the time steps were determined (fixed, free) but the differences were not judged to be significant.
**Solver Manager**

**Click Store Solution**

**Initial Value Tab**
- **Initial Value**
  - Click *Initial value expression evaluated using stored solution*
- **Fixed solution/Linearization point**
  - Click *Stored Solution*

**Solve for Tab**
- **Geom(2D)**
  - *Convection and Diffusion* (highlight)

**Output Tab**
- **Geom 2D**
  - *Incompressible Navier-Stokes* (highlight)
  - *Convection and Diffusion* (highlight)

**Solve**
- Click *Solve Problem*

**Time of Solution : 677.9 sec  Degrees of Freedom  100,088**

**Postprocessing**

The solution to the steady state ns equation and the transient cd equation can be viewed in a number of ways in the postprocessing step. Figure 10 shows the concentration of the tracer after 222 sec at which point the tracer is just reaching the exit. This is consistent with a similar plot presented by Maderia et. al., 2004.

Enter Femlab:

**Postprocessing**
- **General Tab**
  - Check *Surface*
Figure 10  Surface tracer concentration for the reservoir after 222 sec  
(Re = 10, L/H = 1)

The cross sectional plots of Figures 6, 7, 8 and 9 were obtained at x =0.0995 m  
(y = 0.02 to 0.03) rather than at x = 0.1 since a bug exists in Version 3.0 (Comsol_c, 2004).

Enter Femlab:

*Postprocessing*
  
  *Cross Sectional Plots*
  
  General (time selected)  
  Line Extension (cross section line data)

**Spreadsheet Calculations**

After the calculation for the cd equation is complete, postprocessing is accessed and boundary  
integration is requested:

Enter Femlab:

*Postprocessing*
  
  *Boundary Integration*
  
  Boundary Selection 6  
  Time (selected)

The integrated concentration at boundary 6 (the exit) is returned on the screen at the  
requested time and is entered manually into the spreadsheet (Appendix A)  
column ‘Cout/Integrated’. The Danckwert’s F curve values (C_{out}/(0.01*Co) are calculated in  
the next column where the 0.01 term is the height of the exit.
The resident-time distribution function

\[ E(t) = \frac{d}{dt} (F(t)) \]  

(2)

is calculated using an average of the forward and backward derivative of the \( F(t) \) values at a particular time (Chapra et al, 1988). Normalizing

\[ E(\theta) = \frac{E(t)}{\tau} \]  

(3)

where the space-time is

\[ \tau = \frac{\text{Area}}{\text{Flow Rate}} = \frac{(0.1)\times(0.1)/(.001\times.01)}{1000} = 1000 \, \text{1/s} \]  

(4)

Figure 11 is a plot of the residence time distribution \((E(\theta) \text{ vs } \theta)\) out to \(\theta = 0.398\). The plot closely matches the results of Madeira et. al., 2004 except that the tail becomes unstable (compare Figure 3).

**Figure 11** Residence time distribution for \(Re = 10, \, L/H = 1\)

**Determination of Reduced Mean Residence Time**

The mean reduced residence time \(\bar{\theta}_r\) is given (Himmelblau et. al. 1968) by

\[ \bar{\theta}_r = \frac{\bar{t}_r}{\tau} = \int_0^\infty \theta E(\theta) d\theta \]  

(5)
where

\[ \tilde{t}_r = \int_0^\infty t \, E(t) \, dt \]  \hspace{1cm} (6)

Since the tail of the RTD was unstable, determination of the area under the curve was broken into two parts: from \( \theta = 0.208 \) to \( \theta = 0.398 \) and from \( \theta = 0.398 \) to \( \infty \). The area of the first part of the curve was determined by using the trapezoidal rule (Appendix A). The trapezoidal rule was also used for the \( \theta \cdot E(\theta) \) curve.

A plot of \( \ln (E(\theta)) \) vs \( \theta \) is shown in Figure 12.

The plot indicates that a curve of the form

\[ E(\theta) = A \exp(-B \cdot \theta) \]  \hspace{1cm} (7)

could approximate the tail of the curve from \( \theta \) from 0.398 to \( \infty \).

The areas of both \( E(\theta) \) and \( \theta \cdot E(\theta) \) curve can then be calculated analytically from the following:
Noting that

\[ \int_{0}^{\infty} E(\theta) \, d\theta = 1 \]  
(8)

the area under the curve from \( \theta = 0.398 \) to \( \infty \) must be 1 - 0.6590 = 0.3410
where the 0.6590 is the area from \( \theta = 0.208 \) to 0.398

From Equation (7)

\[ \int_{0.398}^{\infty} A \exp\left(-B\theta\right) \, d\theta = \left(\frac{A}{B}\right) \exp\left(-B\times0.398\right) = 0.3410 \]  
(9)

From the spreadsheet at \( \theta = 0.398 \)

\[ E(\theta) = 1.1875 = A \exp\left(-B\times0.398\right) \]  
(10)

Using Equations (9) and (10)

\[ B = \frac{1.1875}{0.3410} = 3.48240 \]  
(11)

and from Equation (7)

\[ A = \frac{1.1875}{\exp(-3.48240\times0.398)} = 4.748579 \]  
(12)
With the values of A and B available the tail of the $\theta * E(\theta)$ curve can be calculated analytically using equation (7):

$$\int_{\frac{1}{398}}^{\infty} \theta E(\theta) \, d\theta = (A/B^2) \cdot (\exp(-0.398*B) \cdot (-B(0.398)-1)) = 0.2337$$  \hspace{1cm} (13)$$

When the tail value is added to the value of the integral calculated in the spreadsheet

$$\text{Total area under } \theta\cdot E(\theta) \text{ curve} = 0.1798 + 0.2337 = 0.4135$$  \hspace{1cm} (14)$$

This compares very well with the value of the mean residence time given by Madeira et al, 2004 of 0.412.
Conclusions

The solution presented in this study is reasonable but could no doubt be improved. The solution presented by Madeira et. al., 2004. (Figure 2) did not appear to require any special processing for the tail and subsequent determination of the mean residence time by integration up to $\theta = 10$. Such a smooth tail could not be generated in this study using the application software.

Madeira et. al., 2004 did mention, however, that a special discretization scheme (Versteeg et. al, 1995) was used for the convective terms.

Madiera et. al., 2004 states “We must point out that to achieve a high level of accuracy, all the simulation results presented in his paper involved a detailed analysis of the numerical algorithms, the mesh employed, and the time step adopted (in transient simulations)” . A similar statement can perhaps be made with regard to Femlab 3.0.

Nomenclature

\[
\begin{align*}
A, B & \quad \text{Parameters in Eq 7} \\
C & \quad \text{Concentration ( kg/m}^3) \\
d & \quad \text{Inlet boundary height (m)} \\
D & \quad \text{Diffusivity (m}^2/\text{s)} \\
E(t) & \quad \text{Resident-time distribution function} \\
E(\theta) & \quad \text{Normalized RTD function, dimensionless} \\
F(t) & \quad \text{Danckwerts’ F curve, dimensionless} \\
H & \quad \text{Height of reservoir, (m)} \\
HH & \quad = H/20 \\
L & \quad \text{Length of reservoir, (m)} \\
Q & \quad \text{Flow rate (m}^2/\text{s)} \\
\text{Re} & \quad \text{Reynolds number, } dU_{\text{mean}} \rho/\eta \\
t & \quad \text{Time (s)} \\
\tilde{t}_r & \quad \text{mean residence time (s)} \\
\text{Umax} & \quad \text{fluid velocity at the center of the inlet boundary (m/s)} \\
\text{Umean} & \quad \text{mean fluid velocity at the inlet boundary (m/s)} \\
u_x & \quad \text{x-velocity (m/s)} \\
u_y & \quad \text{y-velocity (m/s)} \\
x & \quad \text{horizontal coordinate (m)} \\
y & \quad \text{vertical coordinate (m)}
\end{align*}
\]
Greek Symbols

$\delta_{id}$ isotropic diffusion tuning parameter
$\eta$ dynamic viscosity (kg/m-s)
$\theta = t/\tau$, reduced time, dimensionless
$\theta_r$ reduced mean residence time, dimensionless
$\rho$ density (kg/m$^3$)
$\tau$ space-time (s)

References


2. Comsol_a, Technical Support, e-mail of 8/27/2004, Case 29001


4. Comsol_c, Technical Support, e-mail of 8/27/2004, Case 29001


Acknowledgement:

The comments of Prof. P. Rony and the comments and help from technical support of Comsol Inc. is appreciated.
### Appendix A – The Spreadsheet

Residence Time Calculations - CEE Spring 2004 p154

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Integration Using trapezoidal rule from 0.208 to 0.398

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1 Chemical Engineering Education, 38, No 2 Spring 2004 pp 154-160