Femlab 3.0: Experiences in Determining RTD

Edward M, Rosen
EMR Technology Group

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) was used to simulate a 2-D reservoir with dimensions L (length) and H (height) in laminar flow and isothermal conditions (see Figure 1).

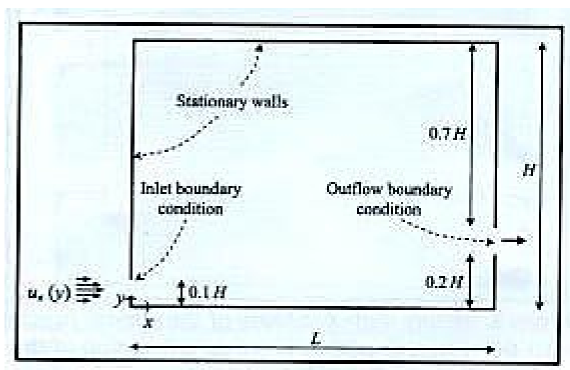


Figure 1 Sketch of Reservoir Geometry

(From Madeira et. al., 2004 with permission)[1]

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

$$u_x = Umax\ [\,1 - \{(y\text{-}H/20)/H/20\}^2]\qquad (1)$$

where

$$Umax = 1.5\ \ Umean$$

There is no slip at the walls ($u_x = u_y = 0$).

A step input of a component with properties similar to water (η = 0.001 kg/(m-s), ρ = 1000 kg/m^3, with D = 5E-10 m^2/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.

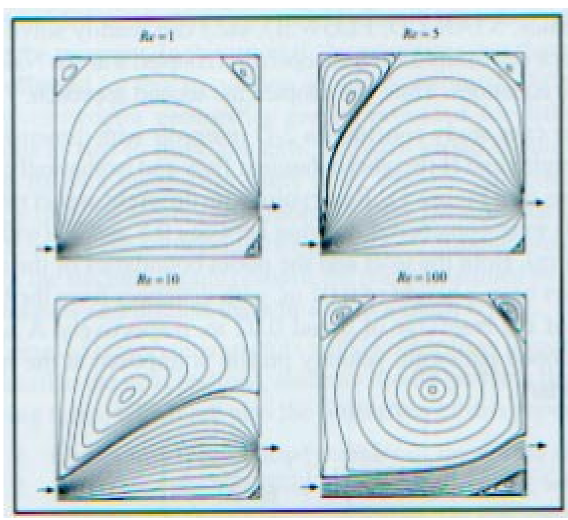


Figure 2. Steady state contours of the stream function for the reservoir with L/H = 1 as a function of Reynolds number

(From Madeira et. al., 2004 with permission)[1]

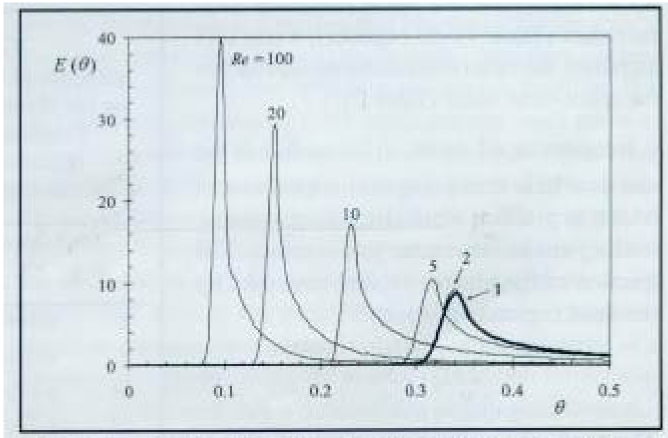


Figure 3 Effect of Reynolds number on the residence
time distribution (L/H = 1)

(From Madeira et. al. 2004 with permission)[1]

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):

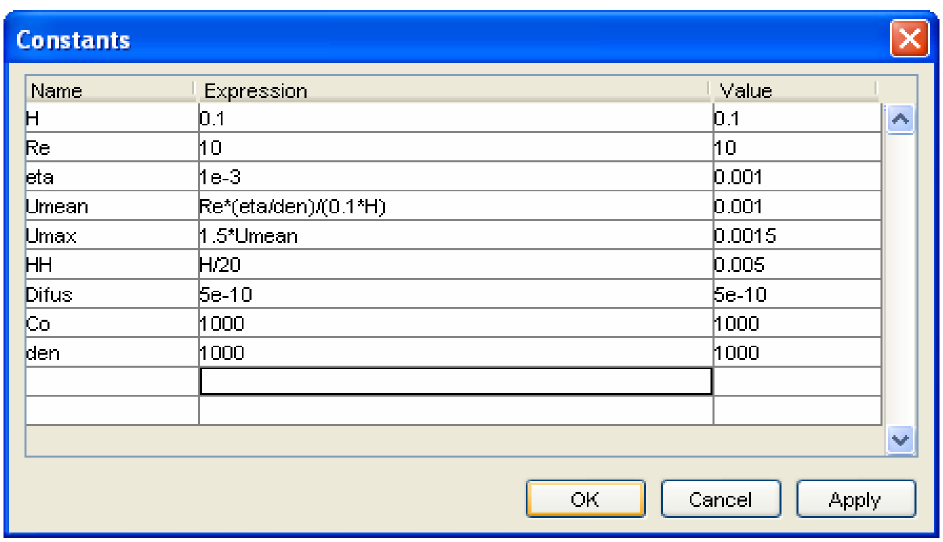
Draw
  Specify Objects
    Line
     Enter the line coordinates for each boundary of the geometry
     Click on *Zoom Extents* (on the menu) after each line is entered.
  Coerce to Solid

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


Constants

Name	Expression	Value
H	0.1	0.1
Re	10	10
eta	1e-3	0.001
Umean	Re*(eta/den)/(0.1*H)	0.001
Umax	1.5*Umean	0.0015
HH	H/20	0.005
Difus	5e-10	5e-10
Co	1000	1000
den	1000	1000

Figure 4. Femlab Constants window

Note (Figure 4) that eta = η, den = ρ, Difus is D (the diffusivity) and Co is the concentration (kg/m^3) of the component at the inlet. Tau (τ) is the space- time and. U_{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

ρ = den Density
η = eta Dynamic Viscosity

Boundary Settings

Boundary Setting 1
Boundary Condition *Inflow/Outflow Velocity*
u_0 *= 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*

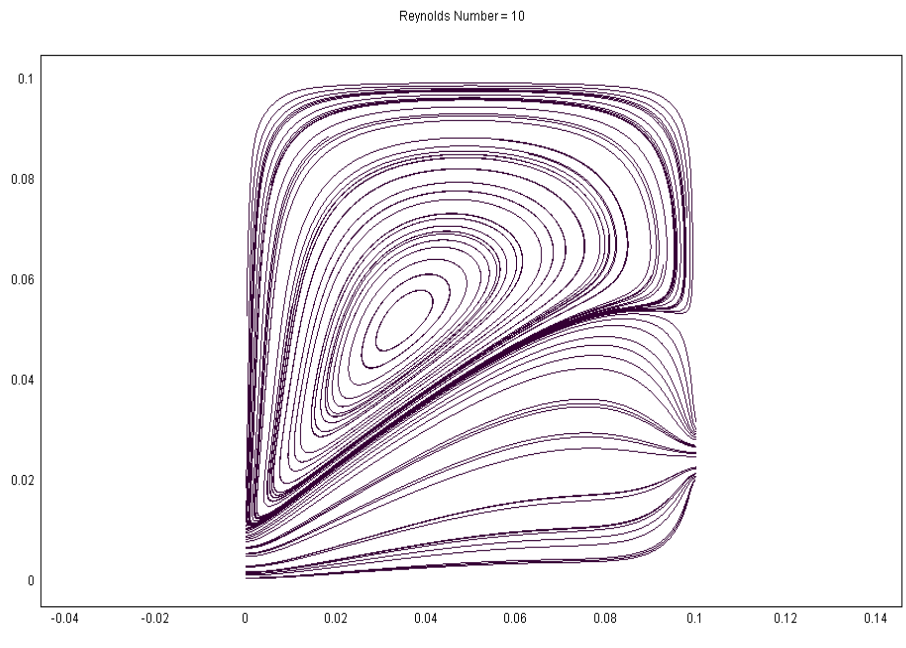


Figure 5 Streamlines of the solution at Re = 10

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.

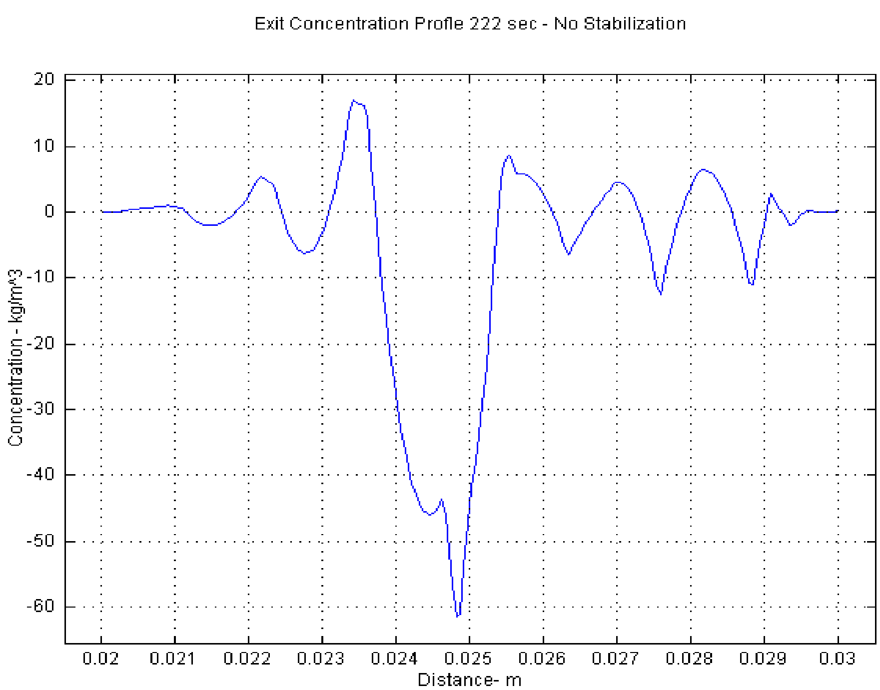


Figure 6. Exit concentration profile at 222 sec with no stabilization

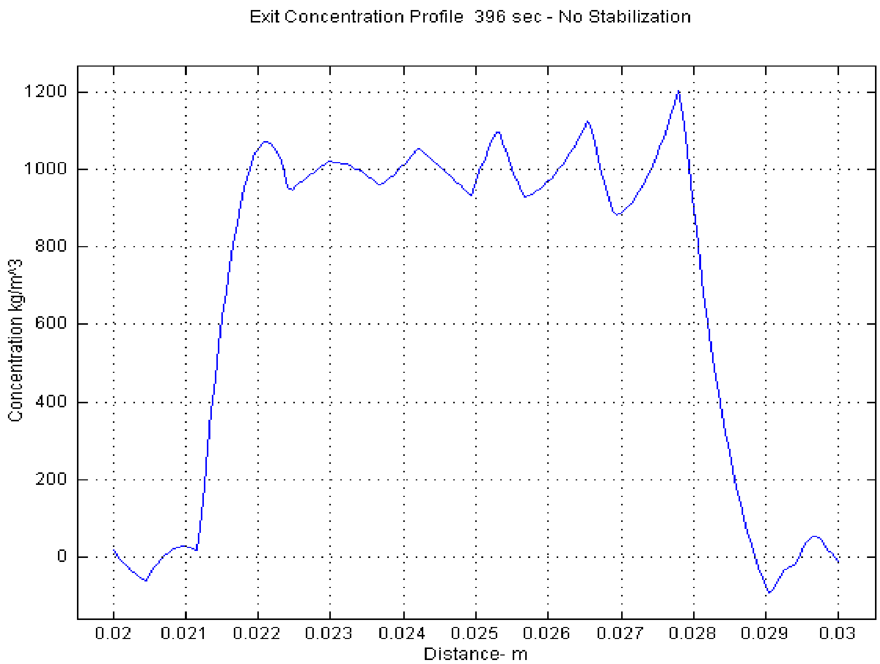


Figure 7 Exit Concentration Profile at 398 sec – No stabilization

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).

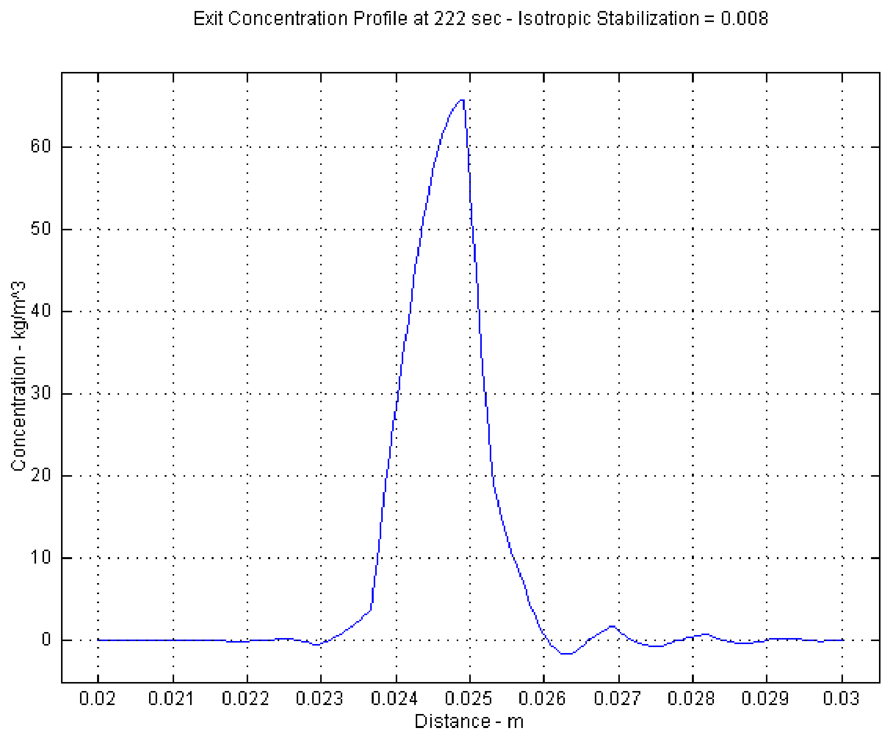


Figure 8 Exit concentration profile at 222 sec with isotropic stabilization = 0.008

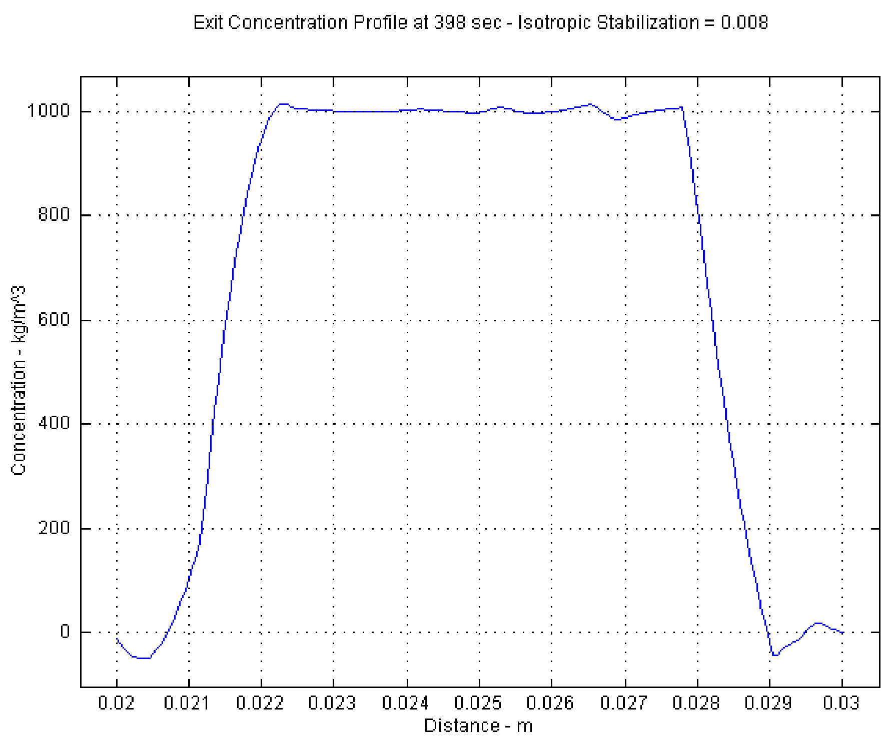


Figure 9 Exit Concentration Profile at 398 sec with isotropic stabilization= 0.008

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

  c Tab

D Isotropic	*Difus*	*Diffusion Coeffiscient*
u	*u*	*x velocity*
v	*v*	*y velcity*

  Artificial Diffusion
    isotropic diffusion δ_{id} = 0.008 *Tuning Parameter*

  Init Tab
    c(t_o) *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*

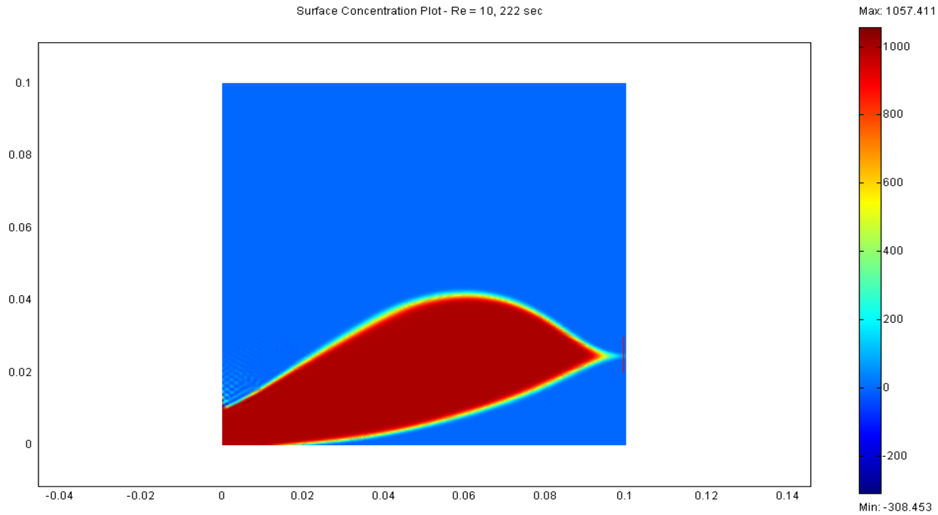


Figure 10 Surface tracer concentration for the reservoir after 222 sec (Re = 10, L/H = 1)

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

$$E(t) = d\,(F(t))/dt \tag{2}$$

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

$$E(\theta) = E(t)/\tau \tag{3}$$

where the space-time is

$$\tau = \text{Area / Flow Rate} = (0.1)*(0.1)/(.001*.01) = 1000\ (1/s) \tag{4}$$

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

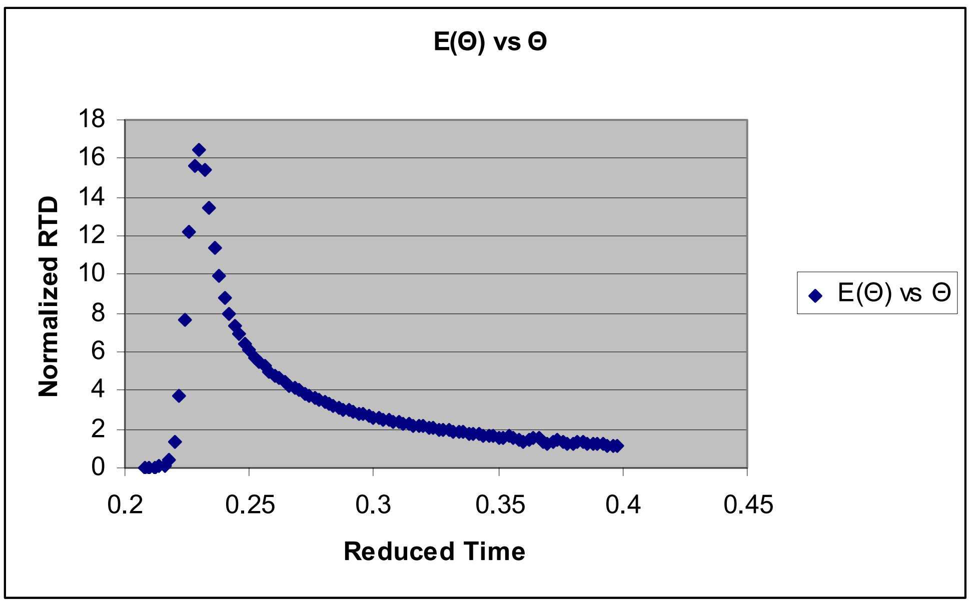


Figure 11 Residence time distribution for Re = 10, L/H = 1

Determination of Reduced Mean Residence Time

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

$$\bar{\theta}_r = \bar{t}_r / \tau = \int_0^\infty \theta E(\theta)\, d\theta \tag{5}$$

where

$$\bar{t}_r = \int_0^\infty t\,E(t)\,dt \qquad (6)$$

Since the tail of the RTD was unstable, determination of the area under the curve was broken into two parts: from θ = 0.208 to θ = 0.398 and from θ = 0.398 to ∞ . 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 θ* E(θ) curve.

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

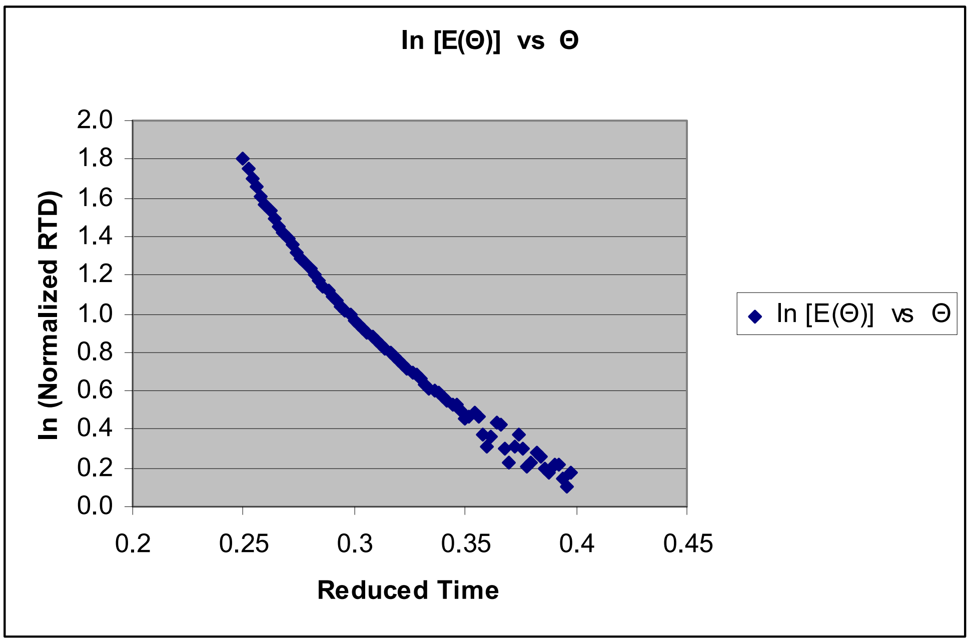


Figure 12. Plot of ln (E(θ)) vs θ

The plot indicates that a curve of the form

$$E(\theta) = A \exp(-B * \theta) \qquad (7)$$

could approximate the tail of the curve from θ from 0.398 to ∞.

The areas of both he E(θ) and θ * E(θ) curve can then be calculated analytically from the following:

Noting that

$$\int_{0}^{\infty} E\,(\theta)\,d\theta \quad = \quad 1 \tag{8}$$

the area under the curve from θ =0.398 to ∞ must be 1- 0.6590 = 0.3410
where the 0.6590 is the area from θ =0.208 to 0.398

From Equation (7)

$$\int_{0.398}^{\infty} \text{A exp (-B* } \theta\text{) d } \theta \quad = \quad \text{(A/B) exp (-B*0.398)} \ = 0.3410 \tag{9}$$

From the spreadsheet at θ = 0.398

$$\text{E(}\theta\text{) = 1.1875 = A exp (-B * 0.398)} \tag{10}$$

Using Equations (9) and (10)

$$\text{B = 1.1875/0.3410 = 3.48240} \tag{11}$$

and from Equation (7)

$$\text{A = 1.1875/exp(-.3.48240*0.398) = 4.748579} \tag{12}$$

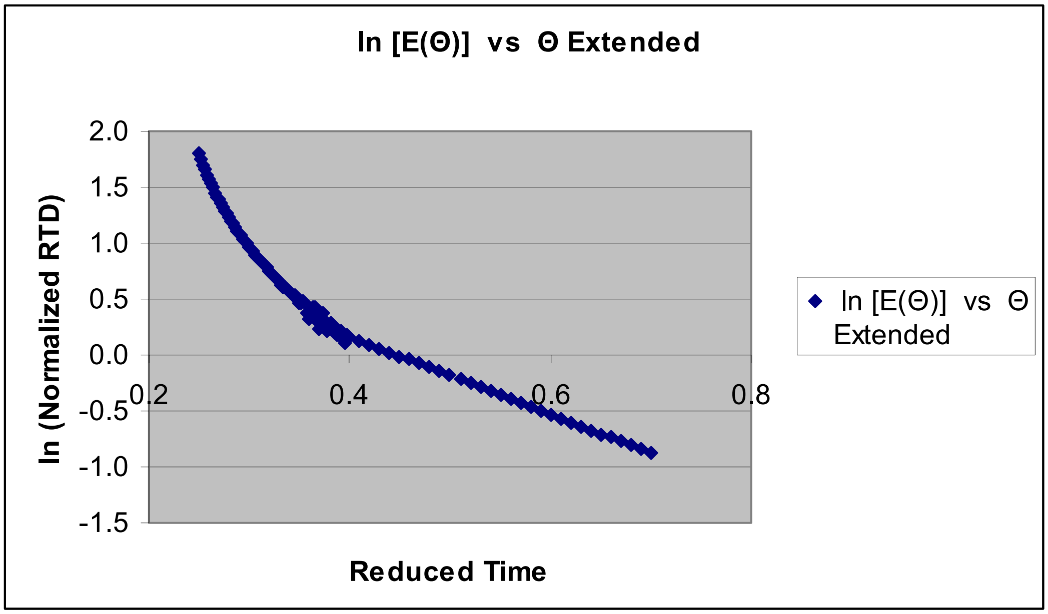


Figure 13 Plot of ln E(θ) vs θ with approximate tail added

With the values of A and B available the tail of the θ * E(θ) curve can be calculated analytically using equation (7):

$$\int_{.398}^{\infty} \theta\, E(\theta)\, d\theta = (A/B^2)*[\,(\exp(-0.398*B) * (-B(.398)-1)] = 0.2337 \qquad (13)$$

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

Total area under θ*E(θ) curve = 0.1798 + 0.2337 = **0.4135** (14)

This compares very well with the value of the mean residence time given my Madeira et el , 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 θ = 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

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

Greek Symbols

δ_{id}	isotropic diffusion tuning parameter
η	dynamic viscosity (kg/m-s)
θ	$= t/\tau$, reduced time, dimensionless
$\bar{\theta}_r$	reduced mean residence time, dimensionless
ρ	density (kg/m^3)
τ	space-time (s)

References

1. Madeira, L. M., M. A. Alves, and A. E. Rodigues, "Teaching Nonideal Reactors With CFD Tools", *Chem. Eng. Ed.*, **38**, 154 (2004)

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

3. Comsol_b, *Femlab 3.0 User's Guide* (January 2004)

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

5. Chapra, S. C. and R. P. Canale, *Numerical Methods for Engineers*, McGraw-Hill, New York (1988)

6. Himmelblau, D. M. and K. B. Bischoff, Process Analysis and Simulation, John Wiley, New York (1968)

7. Verseeg, H. K. and W. Malalasekera, *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*, Prentice Hall, New Jersey (1995)

.

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

τ	1000	δ_{id}	0.008
C_0	1000		

Time sec	$\theta = t/\tau$	Cout Integrated	F(t) = Cout/(0.01*C_0)	E(t)	E(θ)	θ* E(θ)	ln [E(θ)]
206	0.206	1.078E-05	1.078E-06				
208	0.208	2.080E-05	2.080E-06	1.700E-06	0.00170	0.00035	-6.3772
210	0.21	7.877E-05	7.877E-06	2.899E-06	0.00290	0.00061	-5.8435
212	0.212	1.368E-04	1.368E-05	1.840E-05	0.01840	0.00390	-3.9955
214	0.214	8.147E-04	8.147E-05	5.508E-05	0.05508	0.01179	-2.8989
216	0.216	2.340E-03	2.340E-04	1.210E-04	0.12098	0.02613	-2.1121
218	0.218	5.654E-03	5.654E-04	3.826E-04	0.38263	0.08341	-0.9607
220	0.22	1.765E-02	1.765E-03	1.347E-03	1.34713	0.29637	0.2980
222	0.222	5.954E-02	5.954E-03	3.695E-03	3.69452	0.82018	1.3068
224	0.224	1.654E-01	1.654E-02	7.641E-03	7.64070	1.71152	2.0335
226	0.226	3.652E-01	3.652E-02	1.224E-02	12.23534	2.76519	2.5043
228	0.228	6.548E-01	6.548E-02	1.566E-02	15.65590	3.56955	2.7508
230	0.23	9.914E-01	9.914E-02	1.643E-02	16.42785	3.77841	2.7990
232	0.232	1.312E+00	1.312E-01	1.538E-02	15.38010	3.56818	2.7331
234	0.234	1.607E+00	1.607E-01	1.345E-02	13.44752	3.14672	2.5988
236	0.236	1.850E+00	1.850E-01	1.134E-02	11.34020	2.67629	2.4284
238	0.238	2.060E+00	2.060E-01	9.909E-03	9.90938	2.35843	2.2935
240	0.24	2.246E+00	2.246E-01	8.823E-03	8.82328	2.11759	2.1774
242	0.242	2.413E+00	2.413E-01	7.991E-03	7.99125	1.93388	2.0783
244	0.244	2.566E+00	2.566E-01	7.376E-03	7.37608	1.79976	1.9982
246	0.246	2.708E+00	2.708E-01	6.891E-03	6.89125	1.69525	1.9303
248	0.248	2.842E+00	2.842E-01	6.450E-03	6.45040	1.59970	1.8641
250	0.25	2.966E+00	2.966E-01	6.055E-03	6.05493	1.51373	1.8009
252	0.252	3.084E+00	3.084E-01	5.739E-03	5.73918	1.44627	1.7473
254	0.254	3.196E+00	3.196E-01	5.483E-03	5.48285	1.39264	1.7016
256	0.256	3.303E+00	3.303E-01	5.240E-03	5.24008	1.34146	1.6563
258	0.258	3.405E+00	3.405E-01	5.004E-03	5.00420	1.29108	1.6103
260	0.26	3.503E+00	3.503E-01	4.799E-03	4.79877	1.24768	1.5684
262	0.262	3.597E+00	3.597E-01	4.621E-03	4.62140	1.21081	1.5307
264	0.264	3.688E+00	3.688E-01	4.450E-03	4.45025	1.17487	1.4930
266	0.266	3.775E+00	3.775E-01	4.283E-03	4.28338	1.13938	1.4547
268	0.268	3.859E+00	3.859E-01	4.131E-03	4.13083	1.10706	1.4185
270	0.27	3.941E+00	3.941E-01	3.996E-03	3.99645	1.07904	1.3854
272	0.272	4.019E+00	4.019E-01	3.871E-03	3.87098	1.05291	1.3535
274	0.274	4.095E+00	4.095E-01	3.747E-03	3.74725	1.02675	1.3210
276	0.276	4.169E+00	4.169E-01	3.633E-03	3.63333	1.00280	1.2901
278	0.278	4.241E+00	4.241E-01	3.532E-03	3.53185	0.98185	1.2618
280	0.28	4.310E+00	4.310E-01	3.434E-03	3.43363	0.96141	1.2336
282	0.282	4.378E+00	4.378E-01	3.330E-03	3.33040	0.93917	1.2031

284	0.284	4.444E+00	4.444E-01	3.228E-03	3.22755	0.91662	1.1717
286	0.286	4.507E+00	4.507E-01	3.133E-03	3.13268	0.89595	1.1419
288	0.288	4.569E+00	4.569E-01	3.048E-03	3.04792	0.87780	1.1145
290	0.29	4.629E+00	4.629E-01	2.971E-03	2.97147	0.86173	1.0891
292	0.292	4.688E+00	4.688E-01	2.900E-03	2.90005	0.84681	1.0647
294	0.294	4.745E+00	4.745E-01	2.831E-03	2.83093	0.83229	1.0406
296	0.296	4.801E+00	4.801E-01	2.763E-03	2.76260	0.81773	1.0162
298	0.298	4.856E+00	4.856E-01	2.695E-03	2.69540	0.80323	0.9915
300	0.3	4.909E+00	4.909E-01	2.631E-03	2.63083	0.78925	0.9673
302	0.302	4.961E+00	4.961E-01	2.570E-03	2.57037	0.77625	0.9441
304	0.304	5.012E+00	5.012E-01	2.515E-03	2.51450	0.76441	0.9221
306	0.306	5.061E+00	5.061E-01	2.462E-03	2.46188	0.75333	0.9009
308	0.308	5.110E+00	5.110E-01	2.410E-03	2.41037	0.74240	0.8798
310	0.31	5.158E+00	5.158E-01	2.359E-03	2.35890	0.73126	0.8582
312	0.312	5.205E+00	5.205E-01	2.309E-03	2.30850	0.72025	0.8366
314	0.314	5.250E+00	5.250E-01	2.261E-03	2.26130	0.71005	0.8159
316	0.316	5.295E+00	5.295E-01	2.218E-03	2.21815	0.70094	0.7967
318	0.318	5.339E+00	5.339E-01	2.177E-03	2.17658	0.69215	0.7778
320	0.32	5.382E+00	5.382E-01	2.133E-03	2.13280	0.68250	0.7574
322	0.322	5.424E+00	5.424E-01	2.087E-03	2.08695	0.67200	0.7357
324	0.324	5.465E+00	5.465E-01	2.044E-03	2.04403	0.66226	0.7149
326	0.326	5.506E+00	5.506E-01	2.008E-03	2.00773	0.65452	0.6970
328	0.328	5.546E+00	5.546E-01	1.973E-03	1.97333	0.64725	0.6797
330	0.33	5.585E+00	5.585E-01	1.931E-03	1.93140	0.63736	0.6582
332	0.332	5.623E+00	5.623E-01	1.882E-03	1.88242	0.62497	0.6326
334	0.334	5.660E+00	5.660E-01	1.842E-03	1.84200	0.61523	0.6109
336	0.336	5.697E+00	5.697E-01	1.822E-03	1.82203	0.61220	0.5999
338	0.338	5.733E+00	5.733E-01	1.809E-03	1.80862	0.61132	0.5926
340	0.34	5.769E+00	5.769E-01	1.775E-03	1.77522	0.60358	0.5739
342	0.342	5.804E+00	5.804E-01	1.726E-03	1.72580	0.59022	0.5457
344	0.344	5.838E+00	5.838E-01	1.702E-03	1.70238	0.58562	0.5320
346	0.346	5.872E+00	5.872E-01	1.699E-03	1.69860	0.58772	0.5298
348	0.348	5.906E+00	5.906E-01	1.647E-03	1.64728	0.57325	0.4991
350	0.35	5.938E+00	5.938E-01	1.579E-03	1.57925	0.55274	0.4570
352	0.352	5.969E+00	5.969E-01	1.588E-03	1.58815	0.55903	0.4626
354	0.354	6.002E+00	6.002E-01	1.628E-03	1.62758	0.57616	0.4871
356	0.356	6.034E+00	6.034E-01	1.587E-03	1.58707	0.56500	0.4619
358	0.358	6.065E+00	6.065E-01	1.453E-03	1.45287	0.52013	0.3735
360	0.36	6.092E+00	6.092E-01	1.368E-03	1.36808	0.49251	0.3134
362	0.362	6.120E+00	6.120E-01	1.440E-03	1.44010	0.52132	0.3647
364	0.364	6.150E+00	6.150E-01	1.549E-03	1.54875	0.56374	0.4374
366	0.366	6.182E+00	6.182E-01	1.525E-03	1.52530	0.55826	0.4222
368	0.368	6.211E+00	6.211E-01	1.351E-03	1.35118	0.49723	0.3010
370	0.37	6.236E+00	6.236E-01	1.258E-03	1.25775	0.46537	0.2293
372	0.372	6.261E+00	6.261E-01	1.361E-03	1.36143	0.50645	0.3085
374	0.374	6.290E+00	6.290E-01	1.447E-03	1.44725	0.54127	0.3697
376	0.376	6.319E+00	6.319E-01	1.355E-03	1.35513	0.50953	0.3039
378	0.378	6.344E+00	6.344E-01	1.236E-03	1.23558	0.46705	0.2115
380	0.38	6.369E+00	6.369E-01	1.258E-03	1.25765	0.47791	0.2292
382	0.382	6.395E+00	6.395E-01	1.326E-03	1.32632	0.50666	0.2824
384	0.384	6.422E+00	6.422E-01	1.299E-03	1.29947	0.49900	0.2620
386	0.386	6.447E+00	6.447E-01	1.216E-03	1.21573	0.46927	0.1953

388	0.388	6.470E+00	6.470E-01	1.196E-03	1.19592	0.46402	0.1789
390	0.39	6.495E+00	6.495E-01	1.245E-03	1.24530	0.48567	0.2194
392	0.392	6.520E+00	6.520E-01	1.246E-03	1.24578	0.48834	0.2198
394	0.394	6.544E+00	6.544E-01	1.155E-03	1.15475	0.45497	0.1439
396	0.396	6.566E+00	6.566E-01	1.114E-03	1.11430	0.44126	0.1082
398	0.398	6.589E+00	6.589E-01	1.187E-03	1.18715	0.47249	0.1716
400	0.4	6.614E+00	6.614E-01				

Integration Using trapazoidal rule from 0.208 to 0.398

	E(Θ)	Θ * E(Θ)
Value of n	95	95
b-a	0.1900	0.1900
f(.208)	0.0017	0.0007
f(.398)	1.1871	0.4725
Sum f(.21)-f(.396)	328.8818	89.6471
Integral	0.6590	0.1798
Tail	0.3410	0.2337
Total	1.0000	0.4135

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