Femlab Models Used to Test Correlations of Evaporation Rates From Surfaces

Scope of Research

- Pesticides sprayed on a field
- Chemicals in an open channel
- Spilled chemicals

Background

- Evaporation of substances depends on:
  - Physical properties of substances – D, ν, ρ
  - Concentration C_o
  - Surface Area
  - Atmospheric conditions
    - Wind speed
    - Approach concentration C_∞

Femlab Solution

- Solved Using Femlab
- Results compared to:
  - Sleicher's article , I&EC Fund. **25** 659 (1986).
    - *Vaporization and Dispersion from a Surface to a Turbulent Boundary Layer*
  - Barry's article, , CEP, , p. 32, Jan. (2005)
    - *Estimation Rates of Spreading and Evaporation of Volatile Liquids*

Setup

- Large field
- Non dimensional variables

$C_\infty = 0$

Mass Flux = 0

Height z = 8.72 m

$z^+ = 4.0 \times 10^4$

C = 0

Convective Flux

Length L = 350 m

C = 1

$L^+ = 1.6 \times 10^6$

Area = 3.0×10^3 m^2

Boundary Conditions

Theory Equations

- Continuity Equation-

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial z} = 0$$

- Equation of Motion for turbulent flow-

$$\bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{v}\frac{\partial \bar{c}}{\partial z} + \frac{\partial \overline{wc}}{\partial z} = D\frac{\partial^2 \bar{c}}{\partial z^2}$$

- Dimensionless Variables-

$$u^+ = \frac{u}{u_*} \qquad x^+ = \frac{u_* x}{\nu} \qquad z^+ = \frac{u_* z}{\nu}$$

Schmidt and Sherwood numbers

- Schmidt number, Sc is ratio of kinematic viscosity to diffusivity

$$Sc = \frac{\upsilon}{D}$$

- Sherwood number Sh_L is dimensionless concentration gradient at a surface

$$Sh_L = \frac{\bar{k}L}{D}$$

- Sherwood number is related to mass flux

$$N = \bar{k}A\left(C_0 - C_\infty\right)$$

Equations used in Femlab

- Governing equation
  - Convection and diffusion
  - Steady-state

$$u^+ \frac{\partial \theta}{\partial x^+} = \frac{1}{Sc} \frac{\partial}{\partial z^+}\left(1 + Sc \frac{\in_m}{\nu}\right)\frac{\partial \theta}{\partial z^+}$$

- Eddy-diffusivity

$$0 < z^+ < 45: \quad \frac{\in_m}{\nu} = \frac{0.00090 z^{+3}}{\left[1 + 0.0067 z^{+2}\right]^{1/2}}$$

$$z^+ \geq 45: \quad \frac{\in_m}{\nu} = 0.4 z^+$$

- u^+ is x-velocity

$$z^+ < 10: \quad u^+ = z^+$$

$$z^+ \geq 10: \quad u^+ = 5.1 + 2.5 \ln\left(z^+\right)$$

Equations used in Sleicher’ s and Barry’ s

- Sleicher- dependent on Schmidt number and field size

$$Sh_x = 0.81\left(Sc * x^+\right)^{1/3}\left[1 + G\left(x^+\right)^{\alpha}\right]$$

$$G = 0.022 + 0.0008\ln\left(Sc\right)$$

$$\alpha = 0.38 + 0.014\ln\left(Sc\right)$$

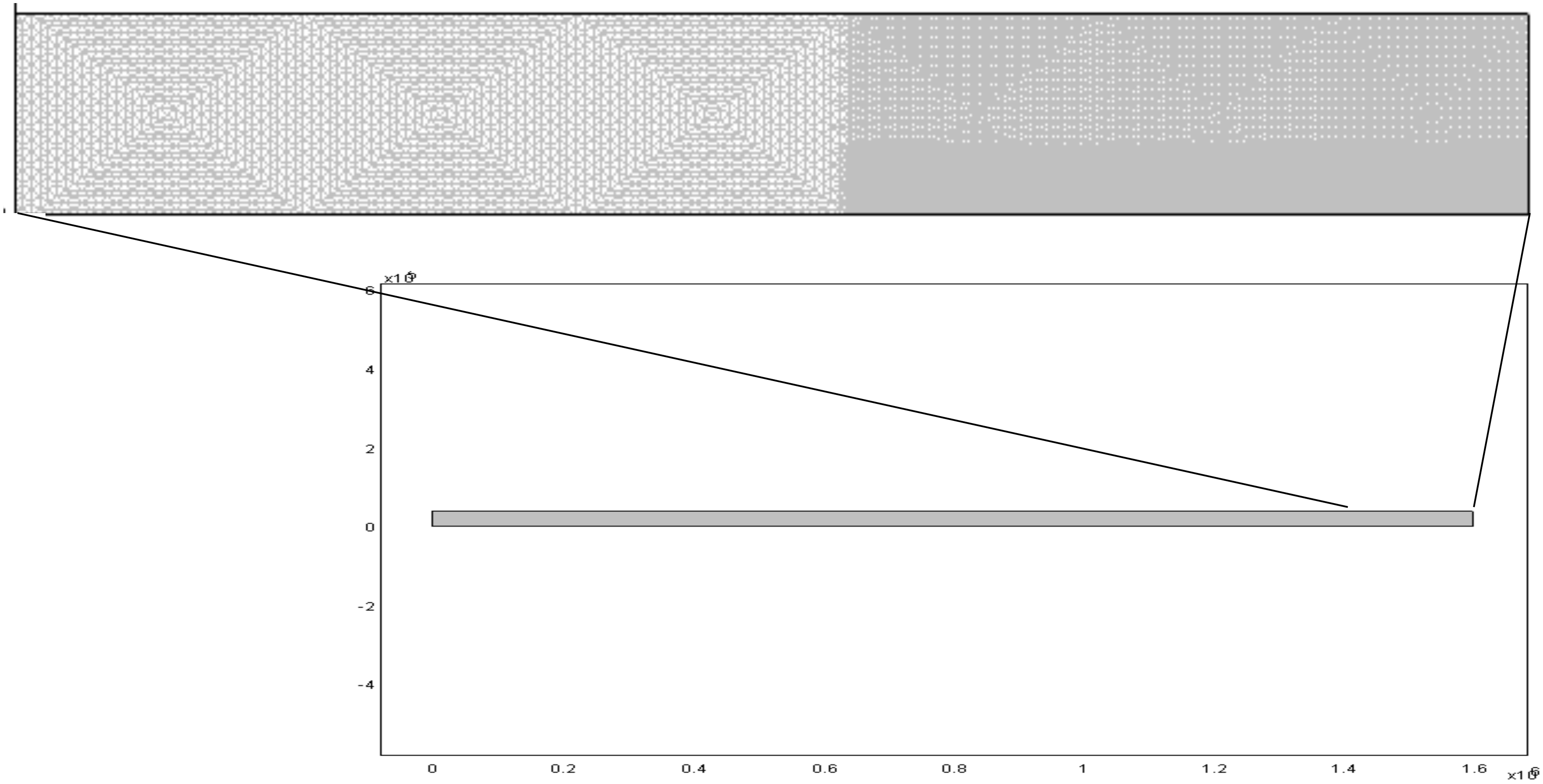
- Barry - dependent on Reynolds number and Schmidt number

$$Sh_x = 0.0365\left(\mathrm{Re}_x\right)^{4/5}\left(Sc\right)^{1/2}$$

$$\mathrm{Re}_x = \frac{u\rho x}{\mu}$$

Mesh Defined

Number of boundary elements	1648
Number of elements	125366
Minimum element quality	0.70
Number of degrees of freedom	252381



Assumptions

- Properties equivalent to air

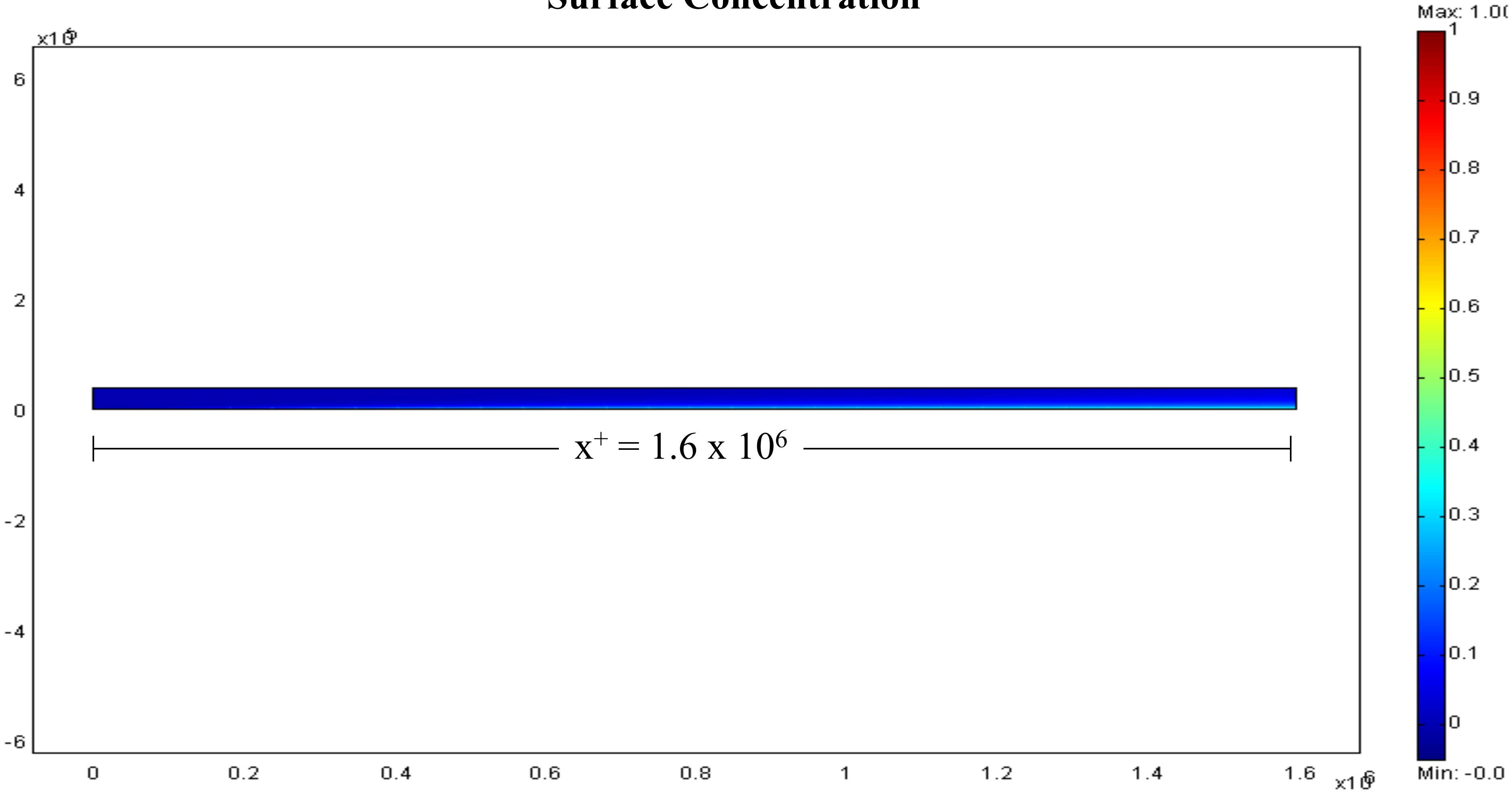
Properties of Substance	
ρ (kg/m3)	1.186
u (m/s)	2
v (m^2/s)	1.57E-05
D (m^2/s)	5.20E-06
μ (kg/ m s)	1.84E-05

Field Properties	
L^+	1.60E+06
z^+	4.00E+04
L (m)	3.49E+02
z (m)	8.72E+00

  - Turbulent Flow Re = 4.51×10^7
- Femlab & Sleicher- Turbulent boundary layer assumption – negligible
- Barry - Turbulent boundary layer regime

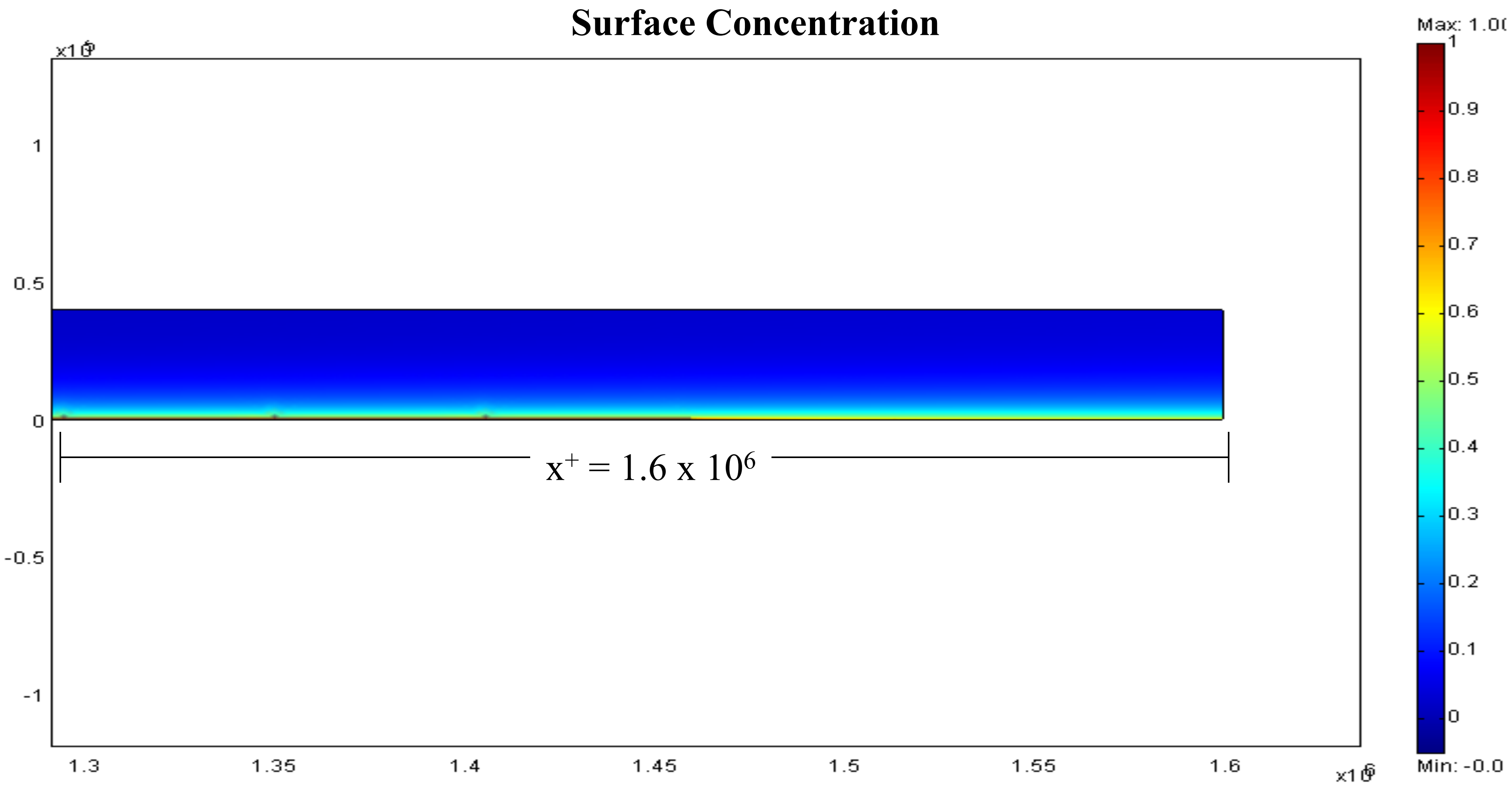
Concentration Profile – Entire Length

Surface Concentration



$x^+ = 1.6 \text{ x } 10^6$

Concentration Profile



Surface Concentration

$x^+ = 1.6 \times 10^6$

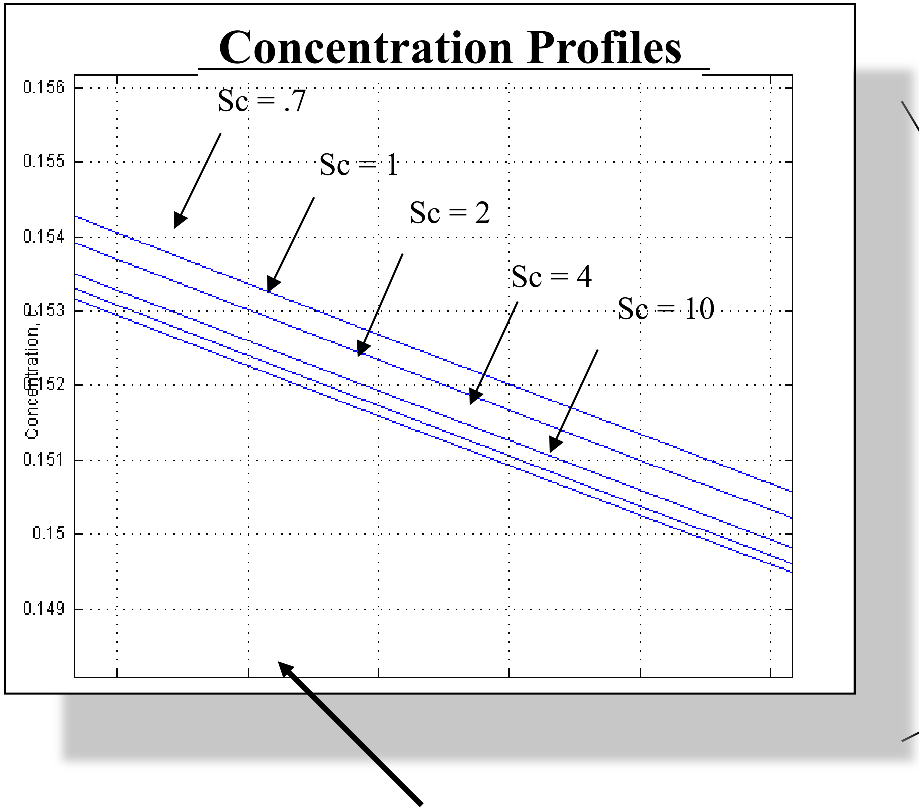
Results – Sherwood numbers

Sherwood numbers at $x^+ = 1.6 \times 10^6$

Sc	Femlab	Barry	Sleicher
0.7	4995	4.05×10^4	426
1	5045	4.85×10^4	570
2	5104	6.85×10^4	980
4	5134	9.69×10^4	1646
10	5153	1.53×10^5	3182

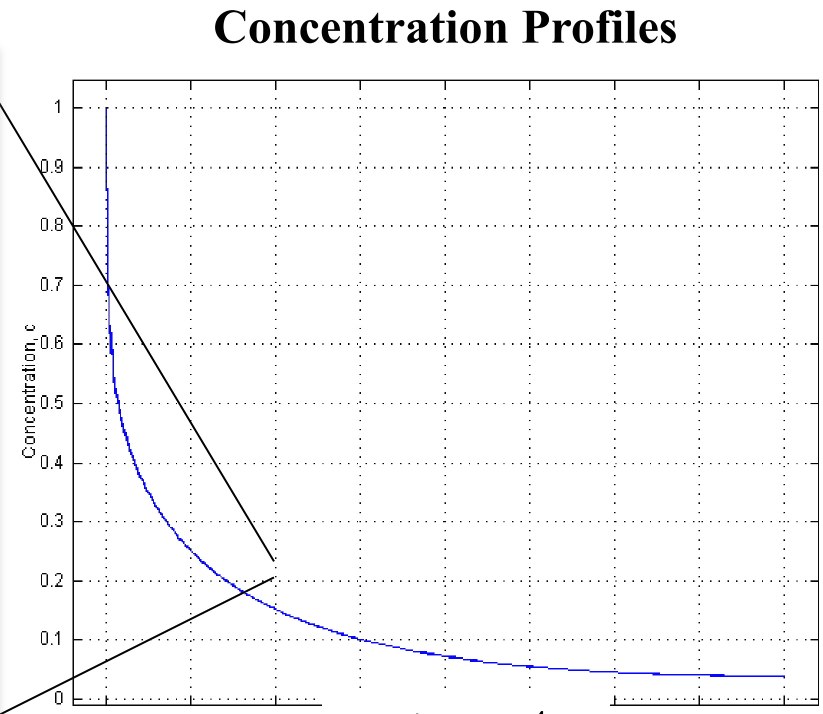
$$Sh_L = \frac{\overline{k}L}{D} \qquad N = \overline{k}A\left(C_0 - C_\infty\right)$$

Varying Schmidt numbers at $x^+ = 1.6 \times 10^6$



$z^+ \times 10^4$

Range: 0.99 – 1.015



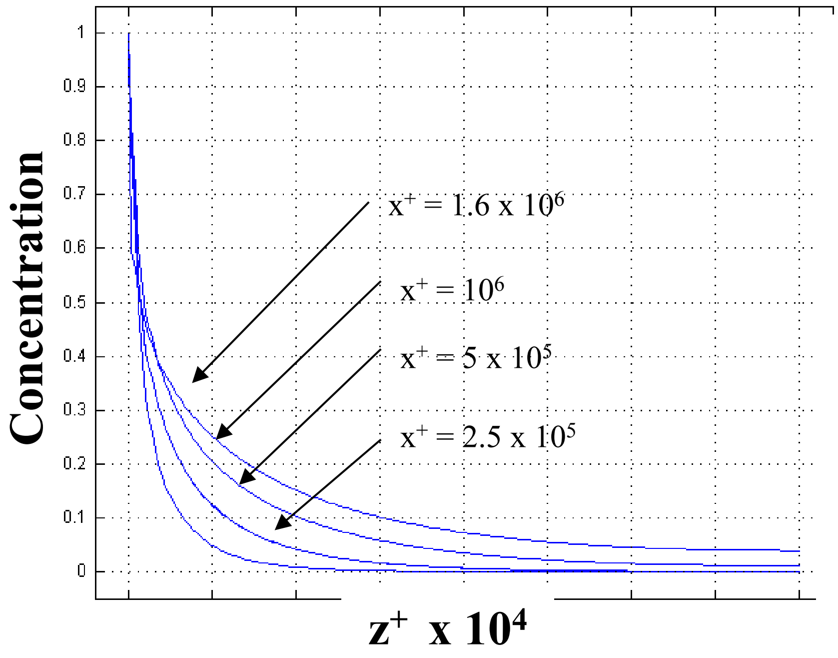
$z^+ \times 10^4$

Range: 0 – 4 x 10^4

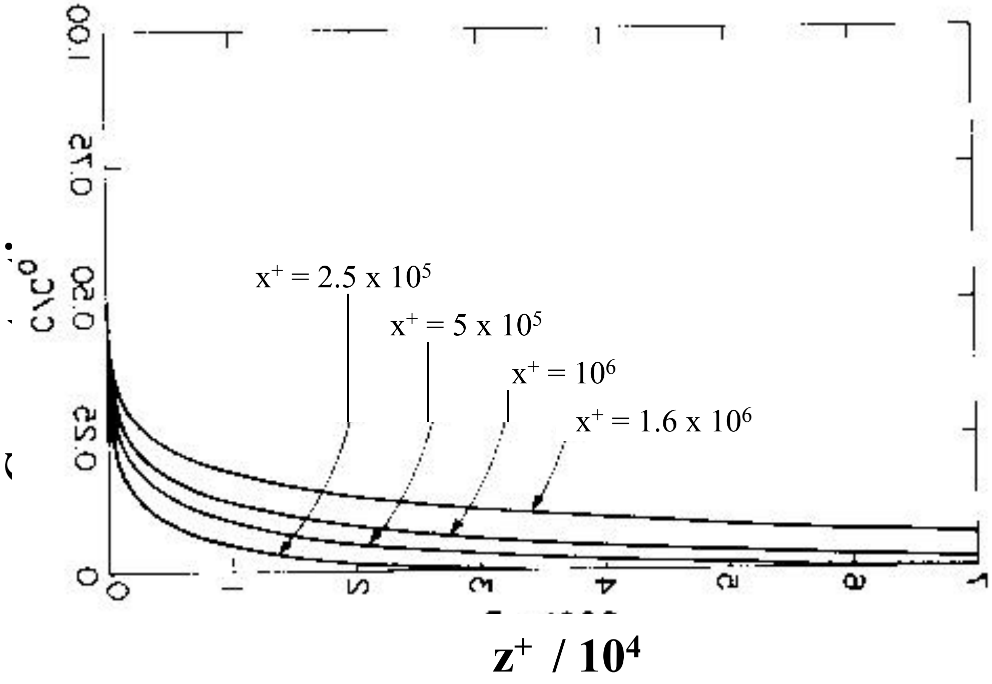
Final Concentrations ~ 5 x 10^{-3}

Concentration Profiles for varying x^+

Femlab Results
Concentration Profile

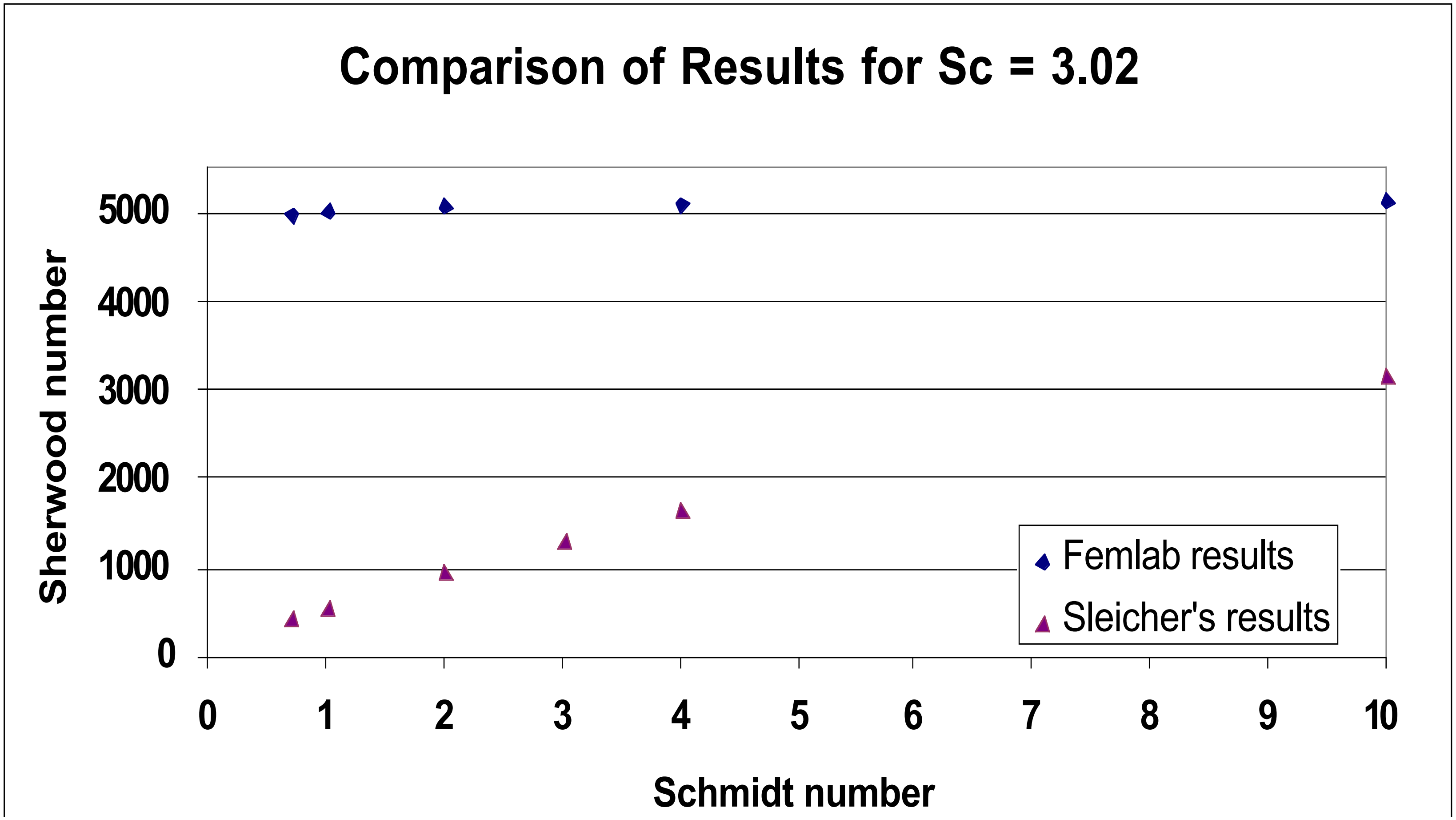


Sleicher's Data
Concentration Profile

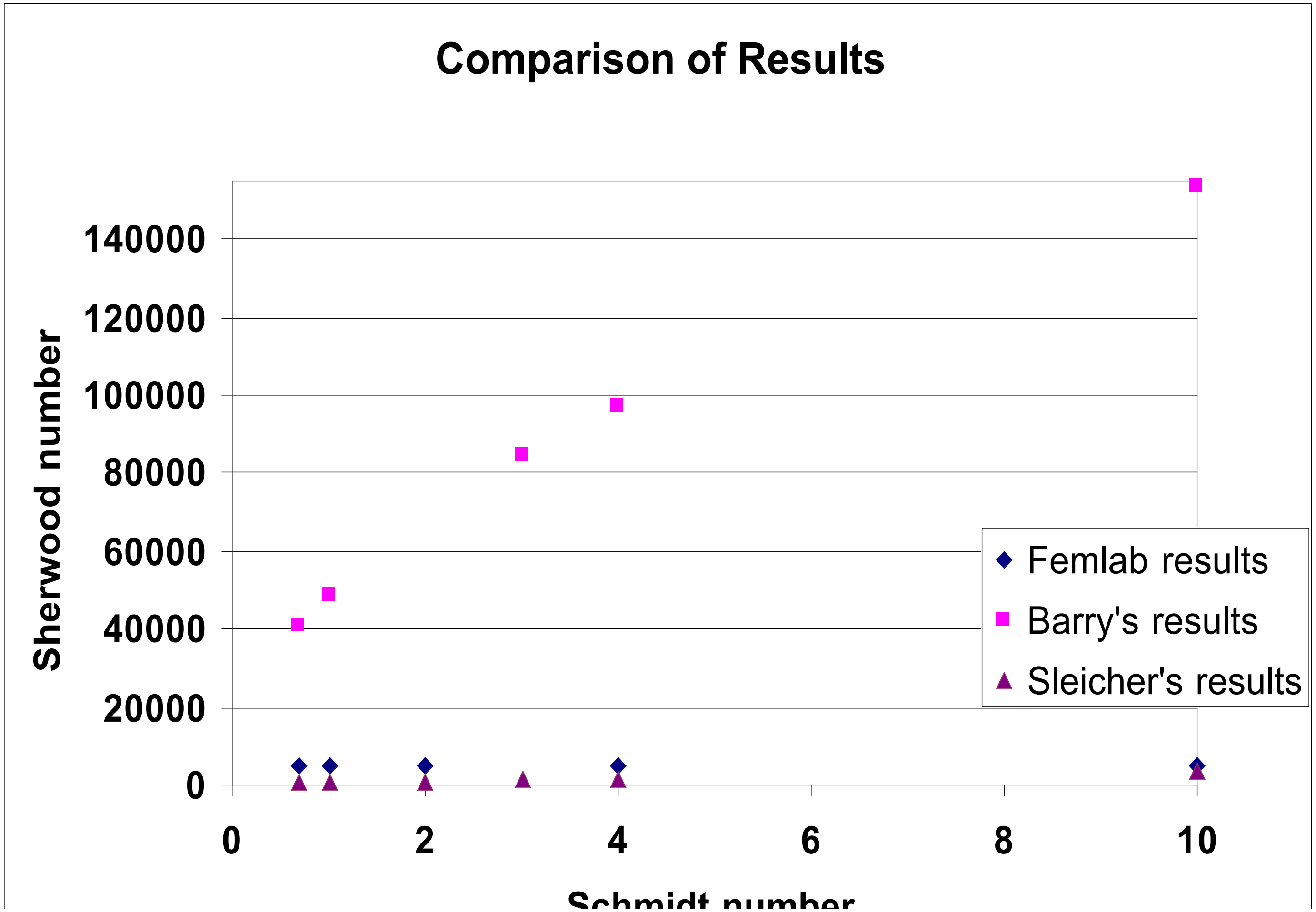


Same Correlation

Femlab vs. Sleicher Comparing Sh_L vs. Sc



Comparing Femlab vs. Barry
Comparing Sh_L vs. Sc



Calculating Sh_x in Femlab

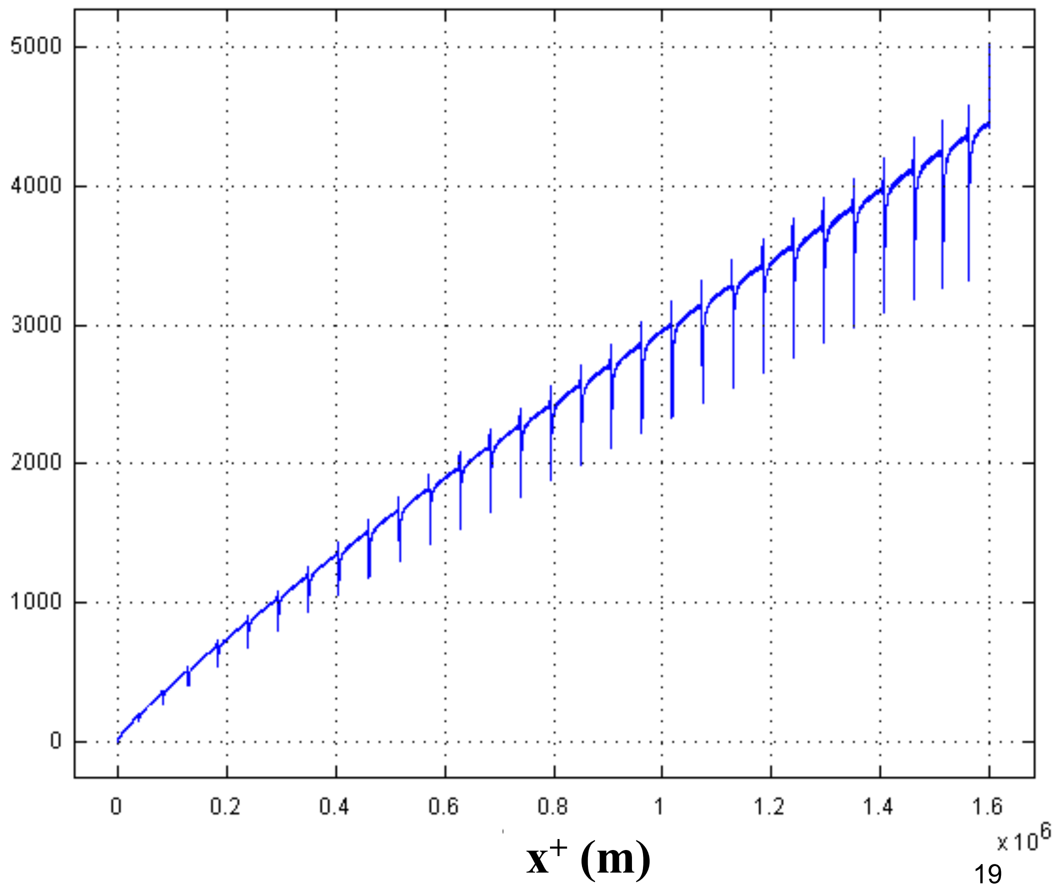
- Relate concentration to Sh_x

$$Sh_x = -x^+ \left.\frac{\partial c}{\partial y}\right|_{z^+=0}$$

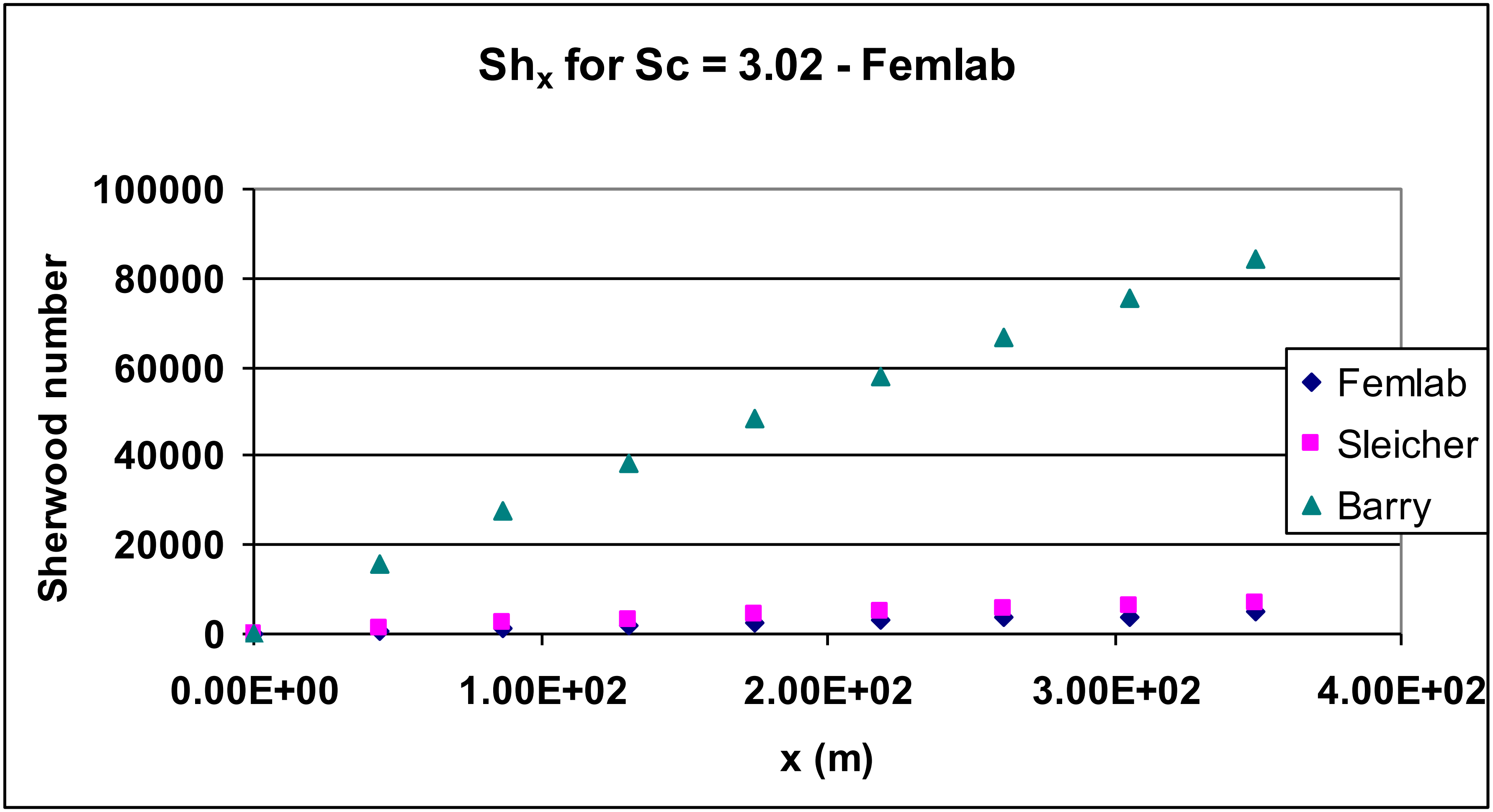
- Relate x^+ to x

$$x^+ = \frac{u_* x}{\nu}$$

Mass Flux



Comparing Sh_x



Discussion

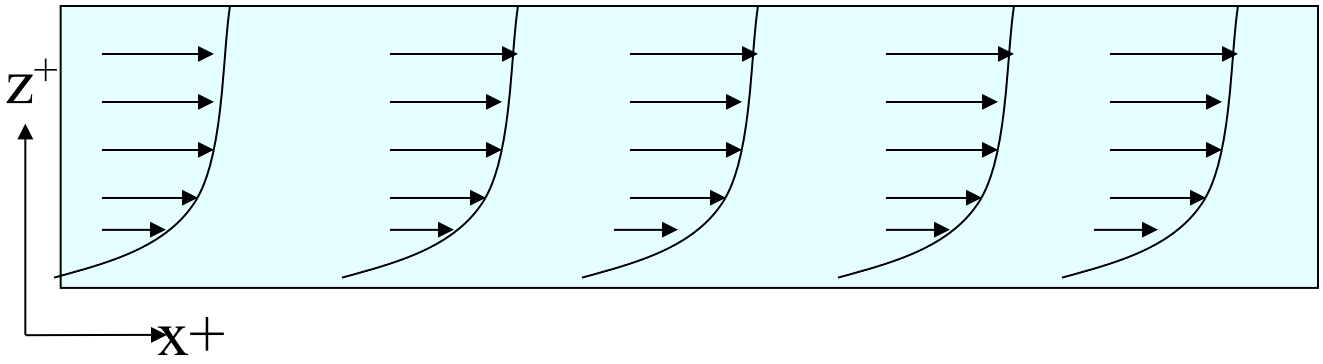
- Comparing Femlab to Sleicher
  - Correlations are the same
  - Not as large of dependence on Sc
  - Sh_L increases faster in Sleicher's equations
- Comparing Femlab to Barry
  - Sherwood numbers VERY different
  - Sh_L increases much faster in Barry's equations

Why the deviations?

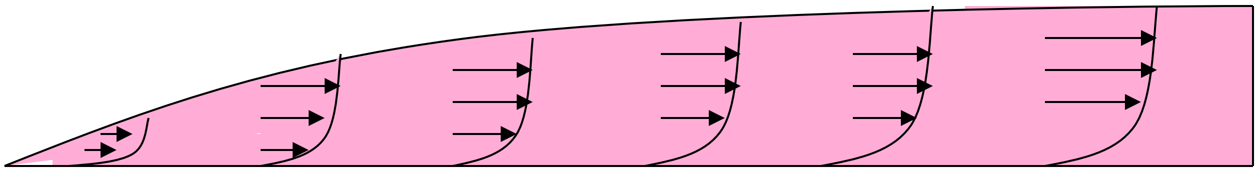
- Sleicher' s numbers are different – factor ~ 1-10
  - Equations are based on empirical data
- Barry' s numbers are different – factor ~ 10-30
  - Equations are based on empirical data
  - Equations apply to turbulent boundary layer
- Femlab solves differential equations analytically

Turbulent Boundary Layer explanation

Femlab = Constant velocity profile



Height z = 8.72 m



Height δ = 3.8 m

Barry = velocity profile ≠ constant

Conclusions

- Femlab accurately models mass flux for turbulent flow
  - Depends on elements and mesh size
- Sleicher’ s equation shows same correlations as Femlab
  - Empirically formed equations
- Barry’ s equation models flow in the turbulent boundary layer regime
  - Empirically formed equations