



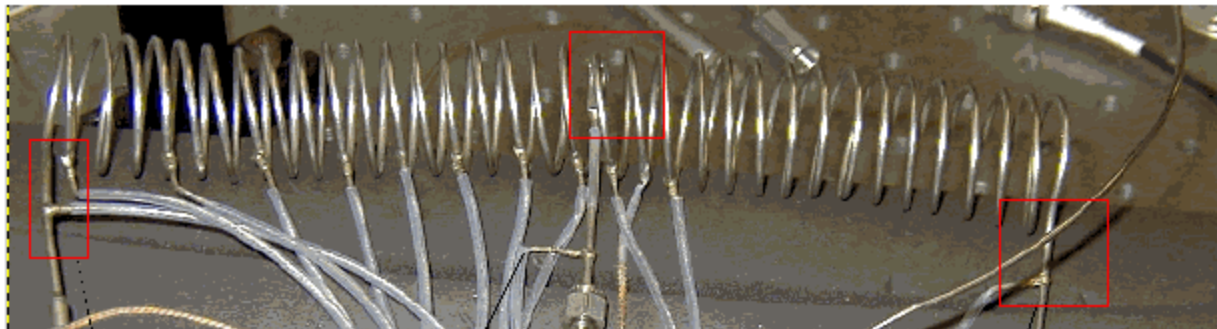
# Mixing in Dow Reactor

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Thursday June 3, 2004

# Introduction

## Dow MicroReactor



Exit

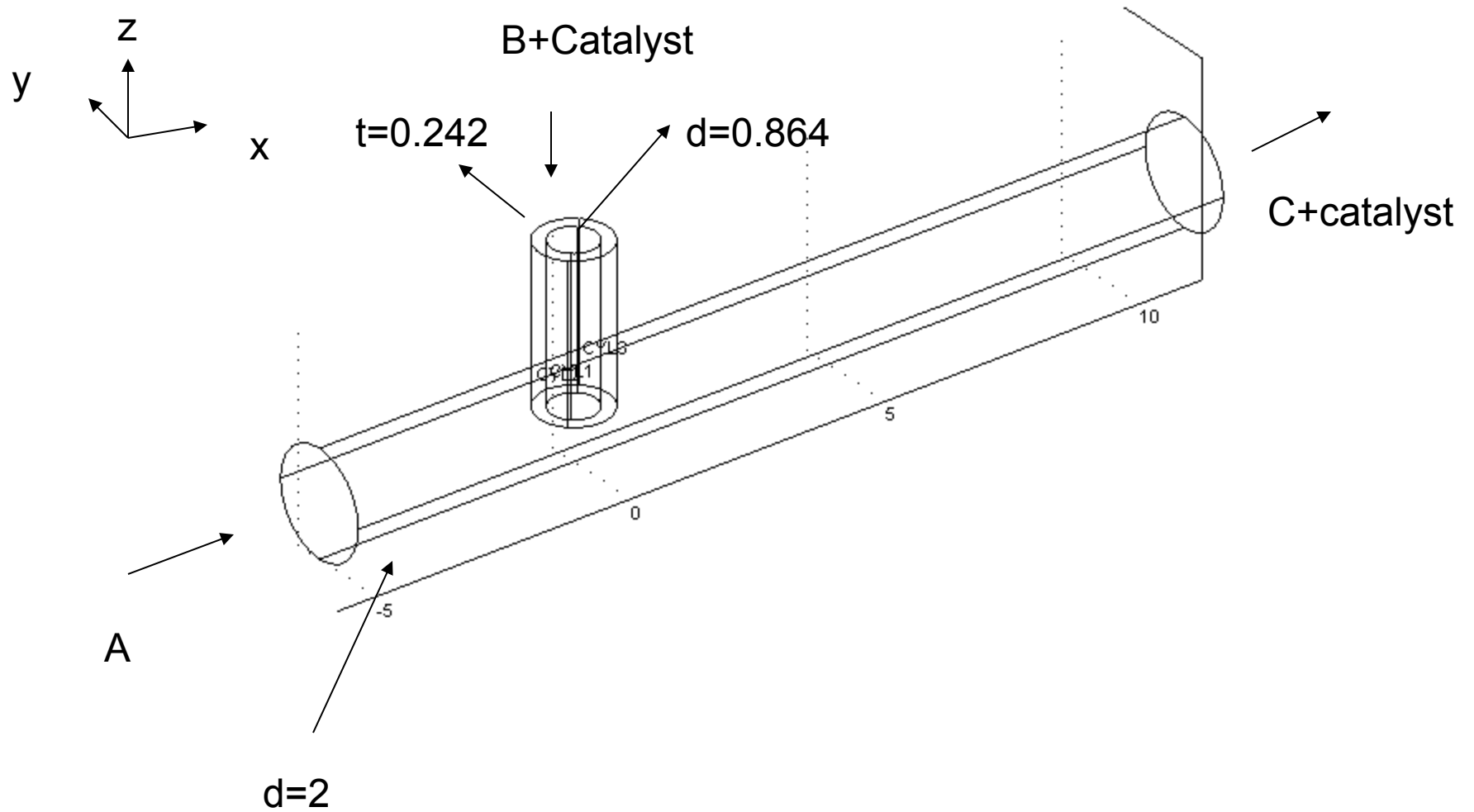
Entrance of  
Liquid B

Entrance of  
Liquid A

# Objective

- Model the 3D Dow reactor in Femlab
- Find the affect of mixing concentration by varying Pe number and rate constant

# Model in Femlab



# Model

## Equation

- Incompressible Navier-Stokes Equation
- Convective Diffusion Equation

## Variable

- Pe number
- Rate =  $k \cdot A \cdot B \cdot \text{catalyst}$

# Boundary Condition

- Navier-Stokes
  - entrance A and B: Parabolic profile velocity
  - exit: straight out
  - wall: no slip
- Convective-Diffusion Equation
  - i. Species A
    - At entrance A;  
Dirichlet  $h=1$   $r=1$
    - At entrance B;  
Dirichlet  
 $h=1$   $r=-$
    - The rest is Neuman
    - Subdomain;  $da=0$ ,  $c=1$ ,  $\beta = 10*u*v*w$ ,  $f=-rate$

# Boundary Condition

## ii. Species B

- At entrance A; Dirichlet  $h=1$ ,  $r=0$
- At entrance B; Dirichlet  $h=1$ ,  $r=1.2$
- The rest are Neuman
- Subdomain;  
 $da=0$ ,  $c=1$ ,  $\beta = 10 \cdot u \cdot v \cdot w$ ,  $f=-2rate$

## iii. Species C

- All boundaries are Neuman
- Subdomain  
 $da=0$ ,  $c=1$ ,  $\beta = 10 \cdot u \cdot v \cdot w$ ,  $f=rate$

# Boundary Condition

## iv. Species D (catalyst)

- At entrance A; Dirichlet  $h=1$ ,  $r=0$
- At entrance B; Dirichlet  $h=1$ ,  $r=0.3$
- The rest are Neuman
- Subdomain;  
 $da=0$ ,  $c=1$ ,  $\beta = 10 \cdot u \cdot v \cdot w$ ,  $f=0$



# Mesh Statistics

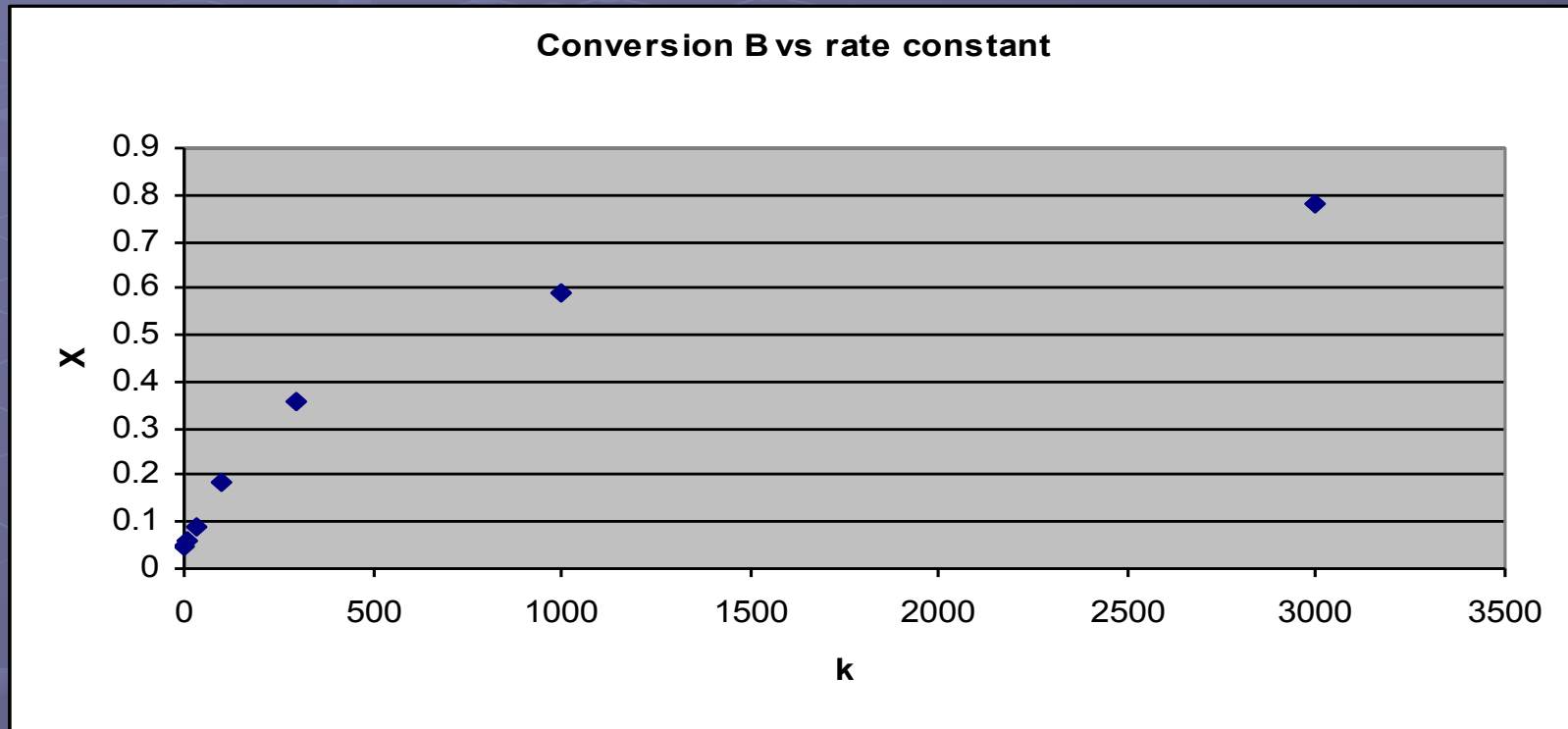
## Extended Mesh

- Number Degrees of Freedom=27797

## Base Mesh

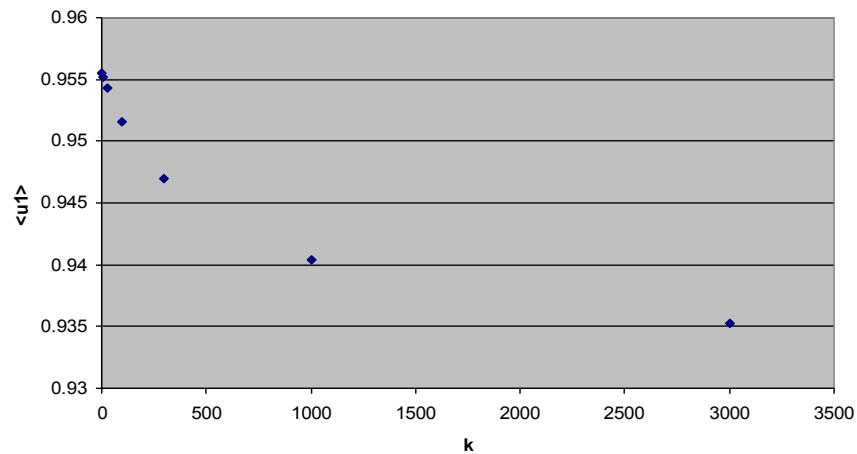
- Number of elements= 3631
- Number of boundary elements = 1502
- Number of edge elements = 270
- Min. element quality = 0.0208

# Result for varying rate constant

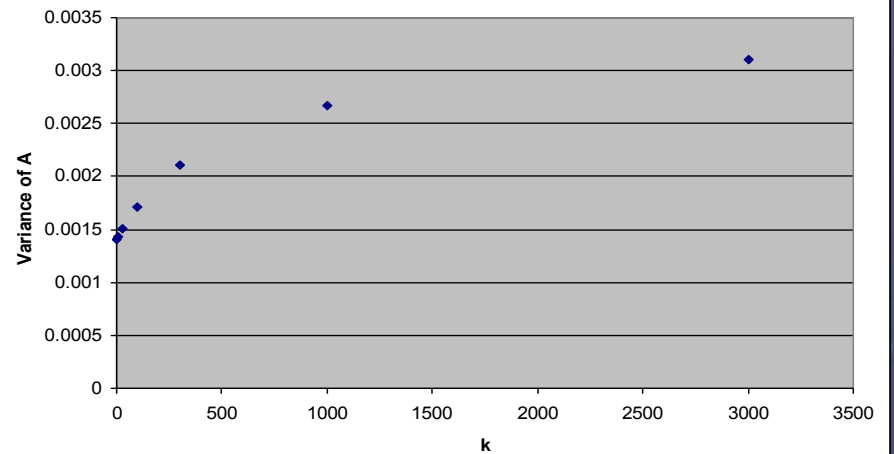


# Result for varying rate constant

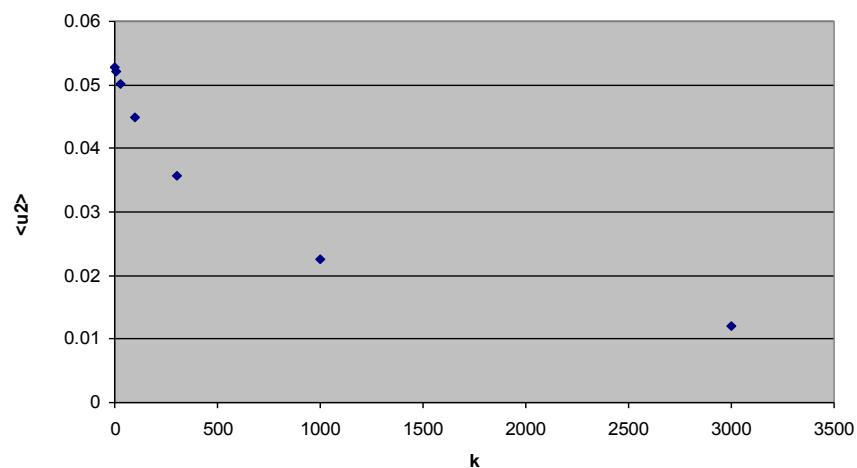
Average Concentration A vs rate Constant



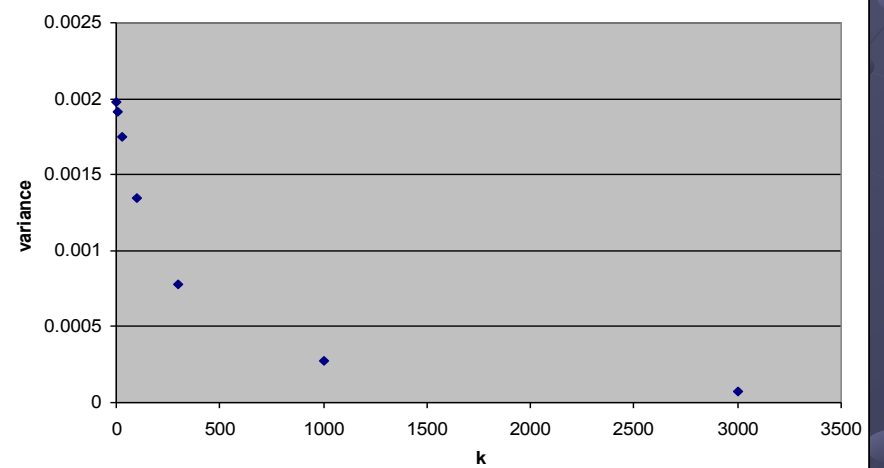
variance A vs rate constant



Avg concentration B vs rate constant

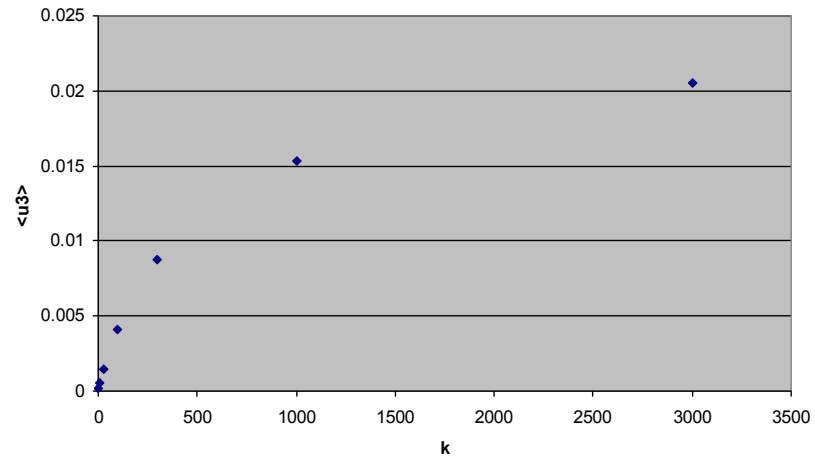


variance B vs rate constant

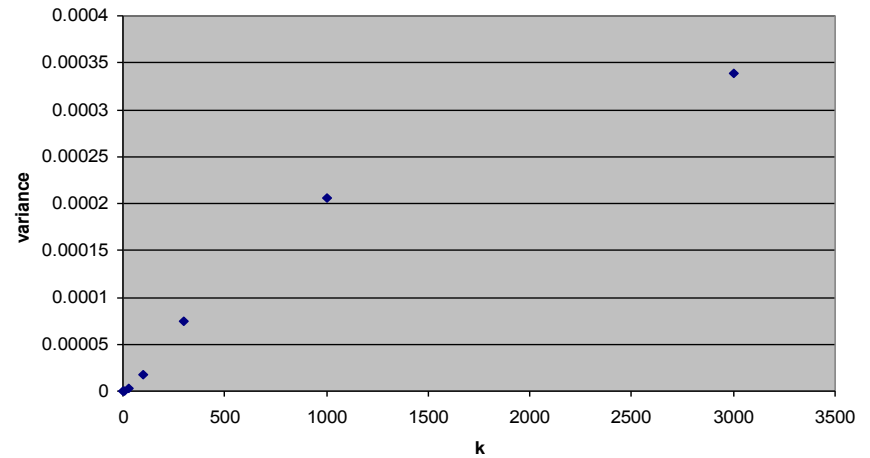


# Result for varying rate constant

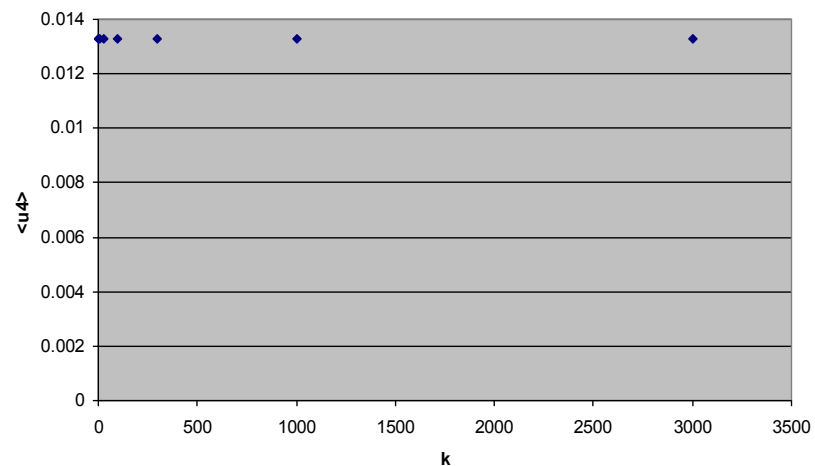
Avg concentration C vs rate constant



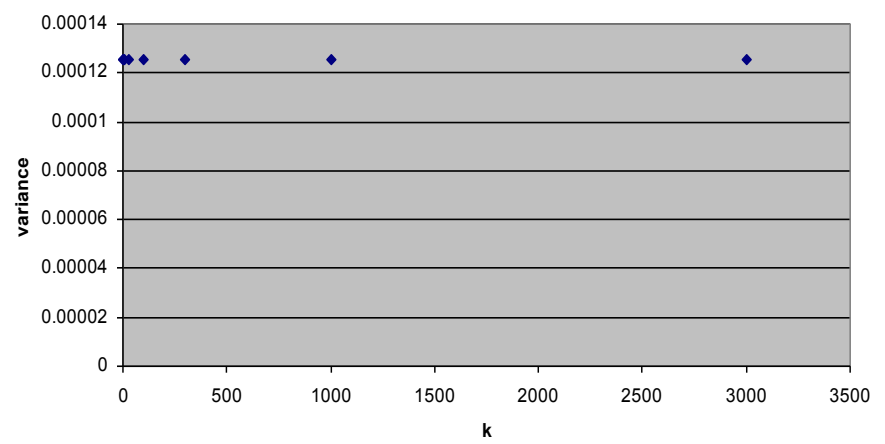
variance C vs rate constant



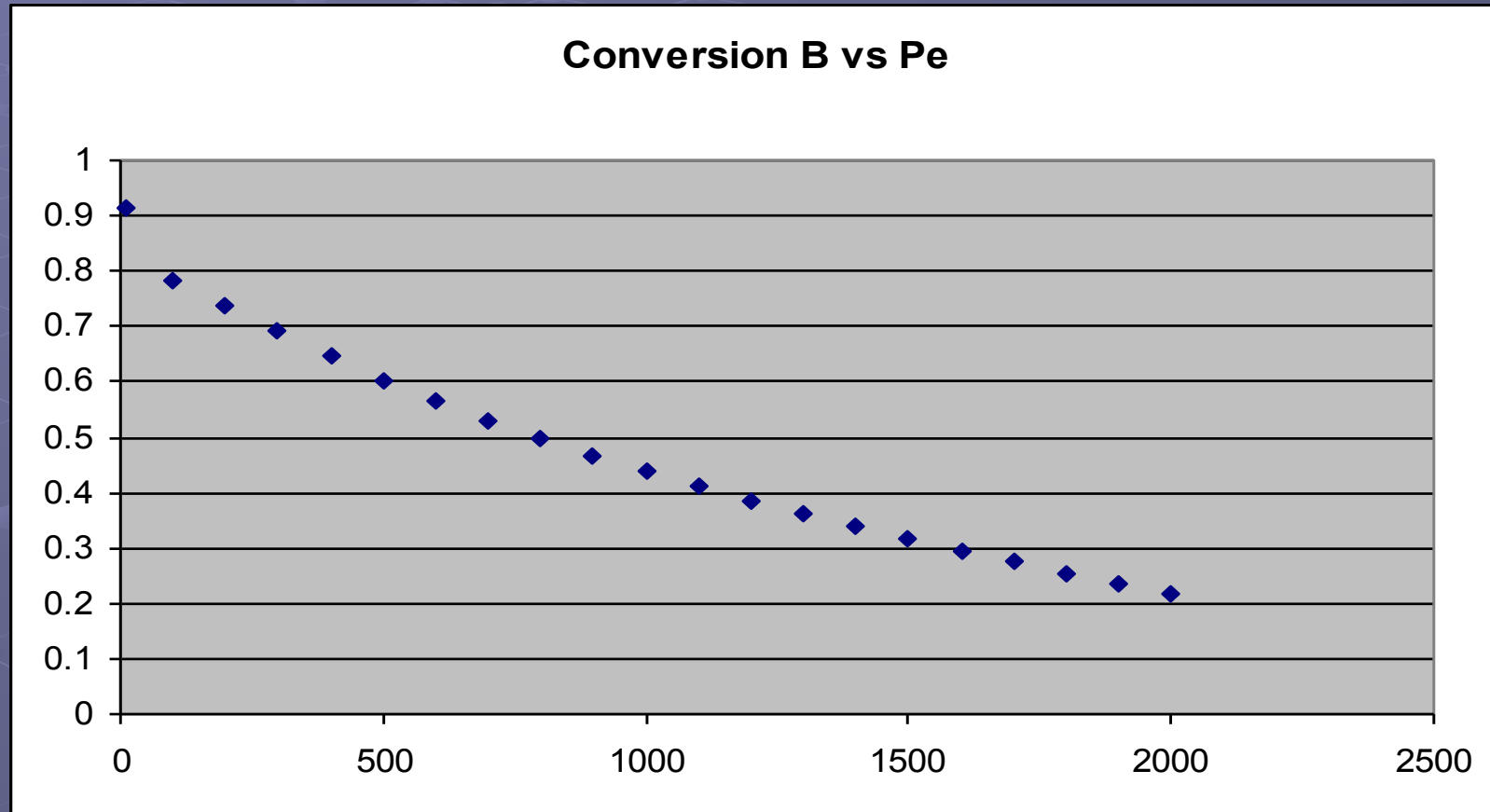
Avg concentration D vs rate constant



variance D vs Rate constant

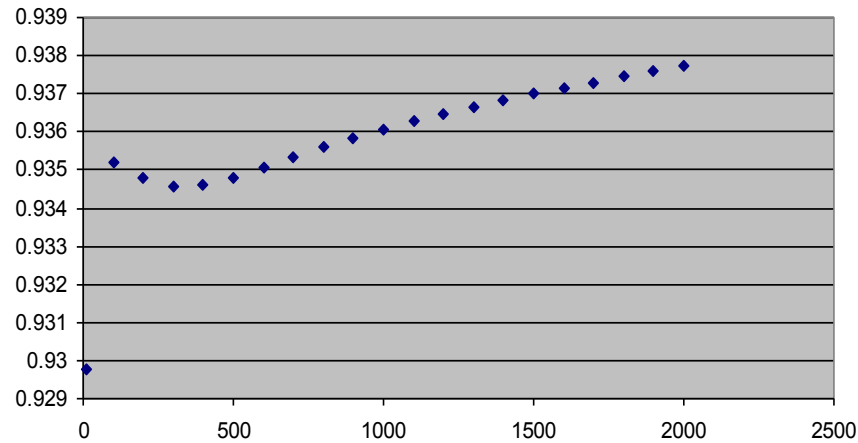


# Result for Varying Pe number

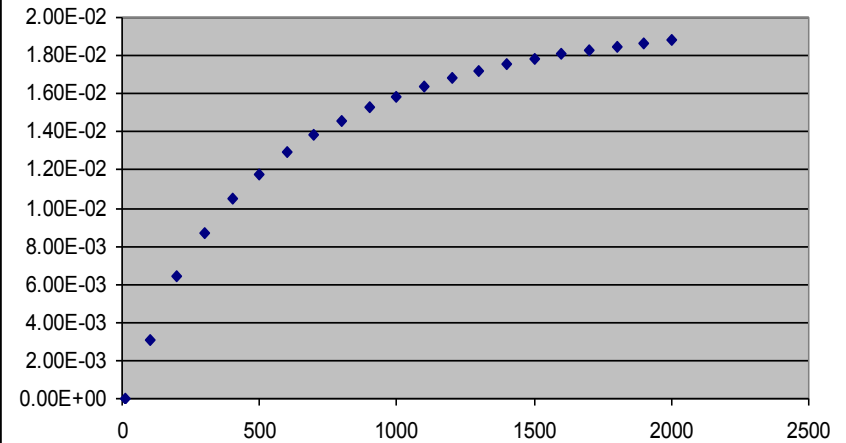


# Result for Varying Pe number

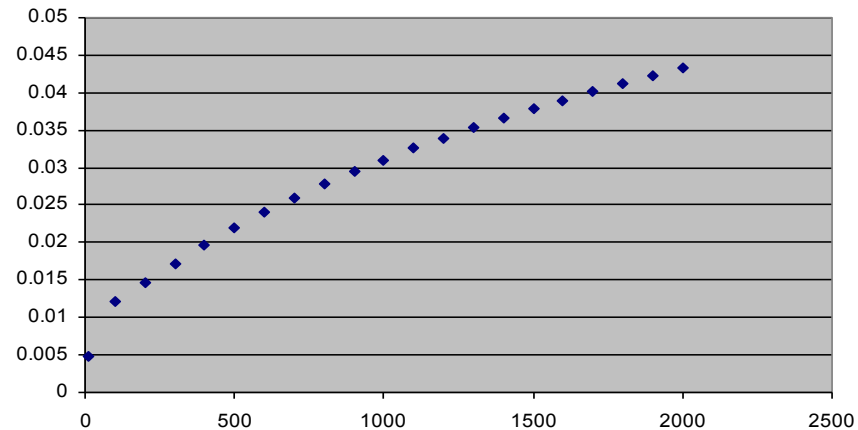
Average Conc. A vs Pe



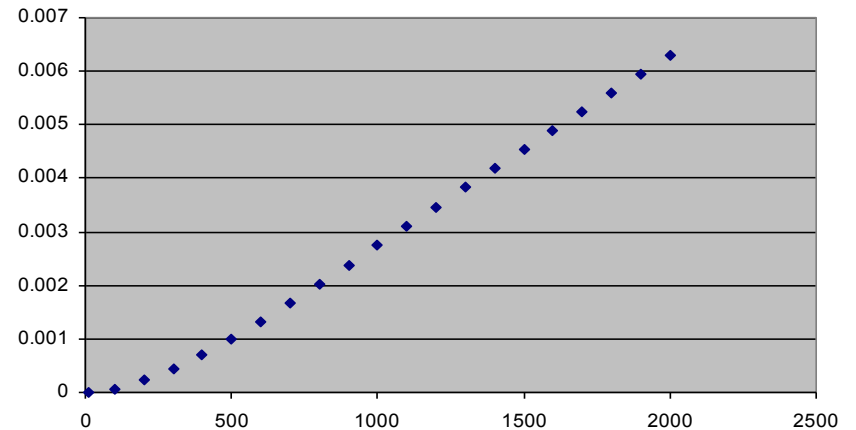
Variance A vs Pe



Avg conc of B vs Pe

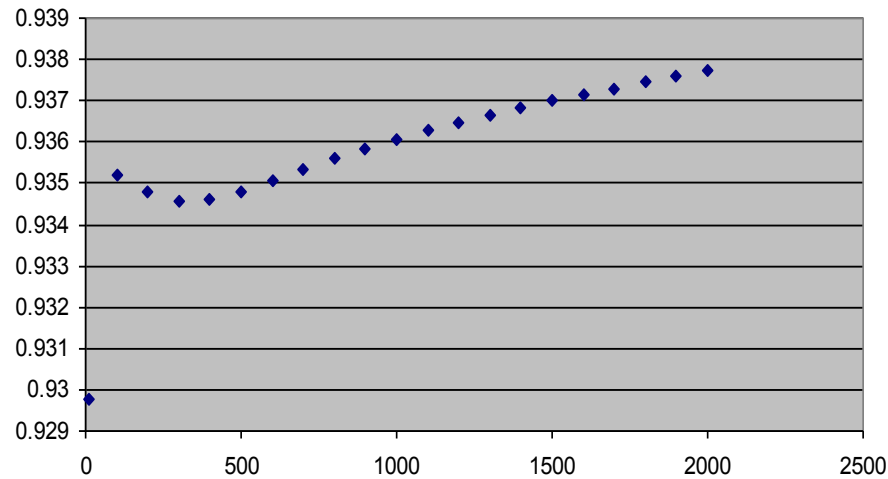


variance of B vs Pe

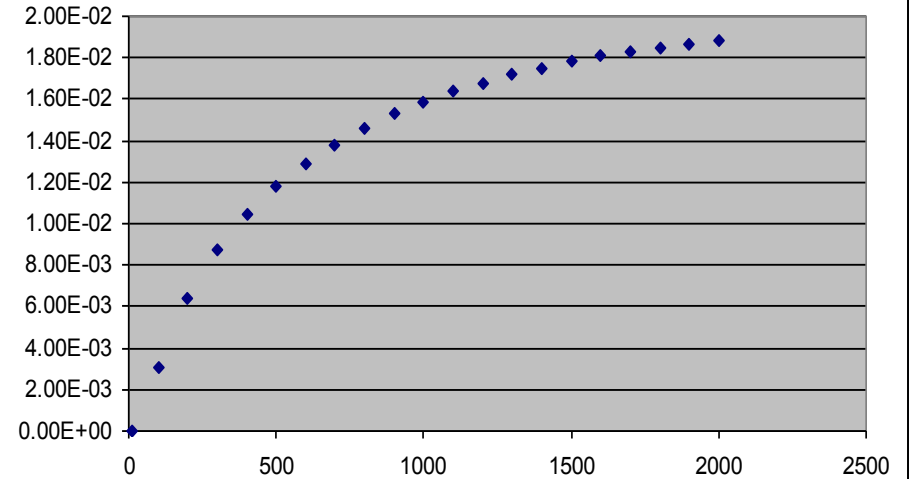


# Result for Varying Pe number

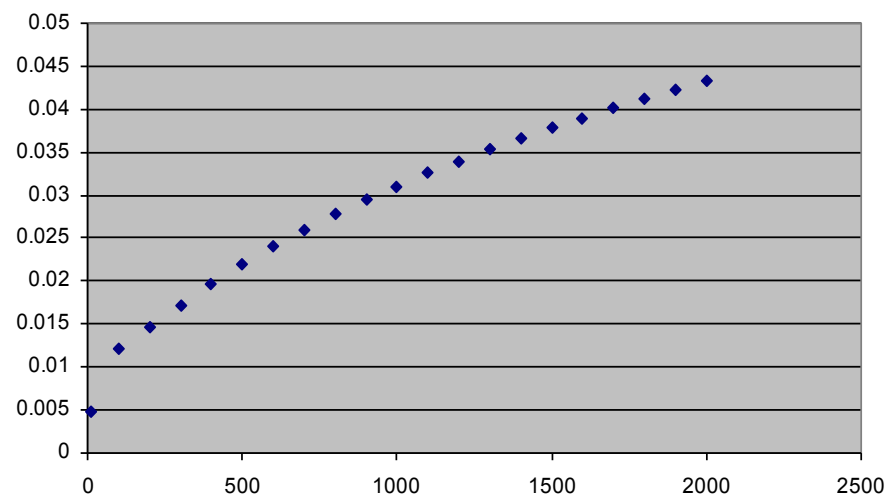
Average Conc. A vs Pe



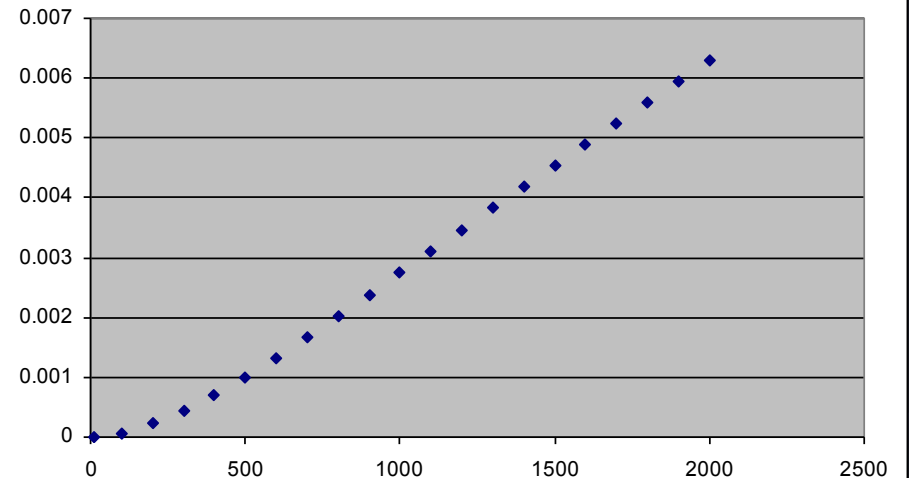
Variance A vs Pe



Avg conc of B vs Pe



variance of B vs Pe

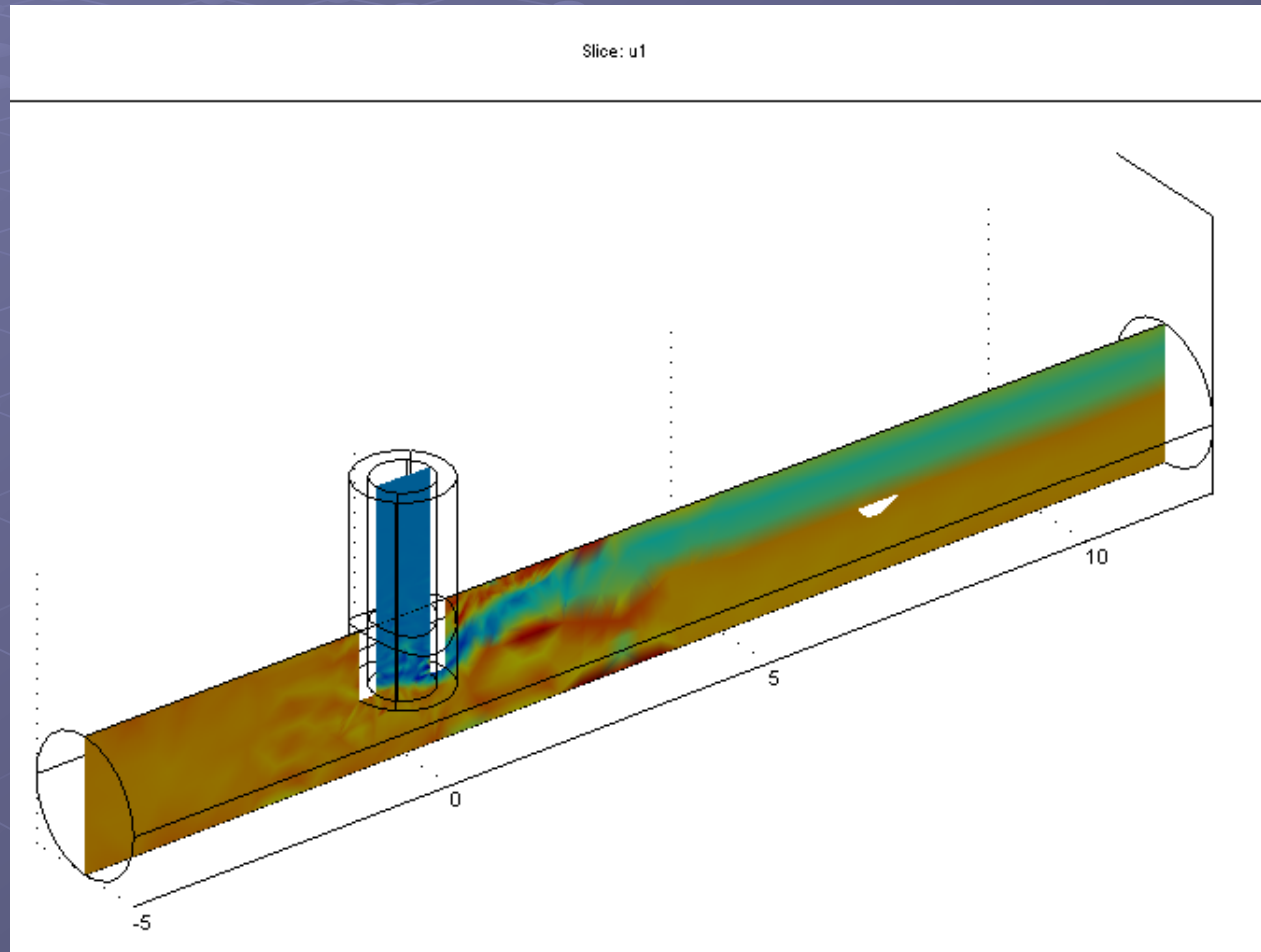


# Rate calculation

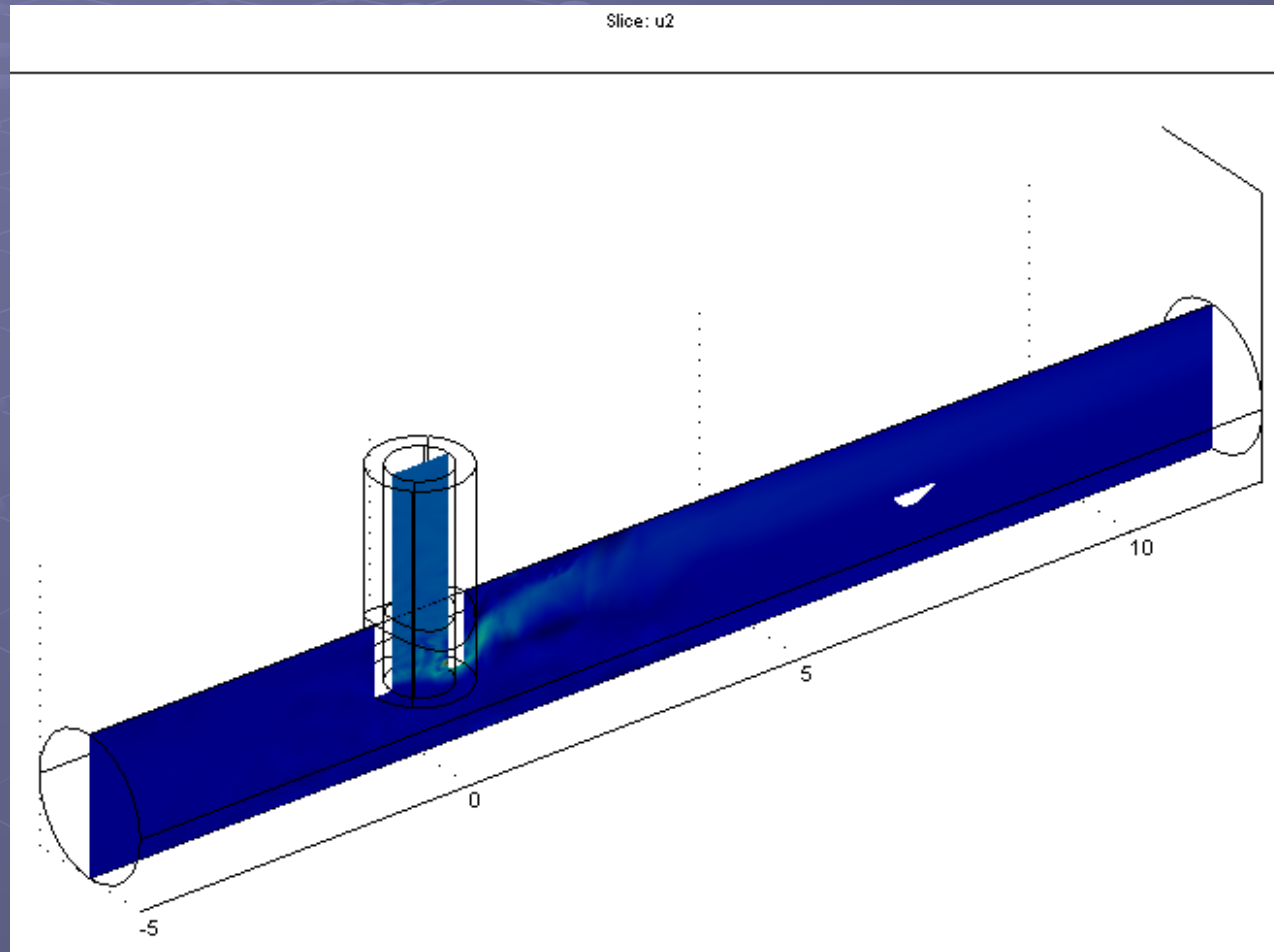
rate integration	Pe 2000	0.945312821
rate by hand		0.082854831
rate integration	Pe 1000	0.397037543
rate by hand		0.040345419
rate by integration	Pe 100	0.012634823
rate by hand		0.008437632



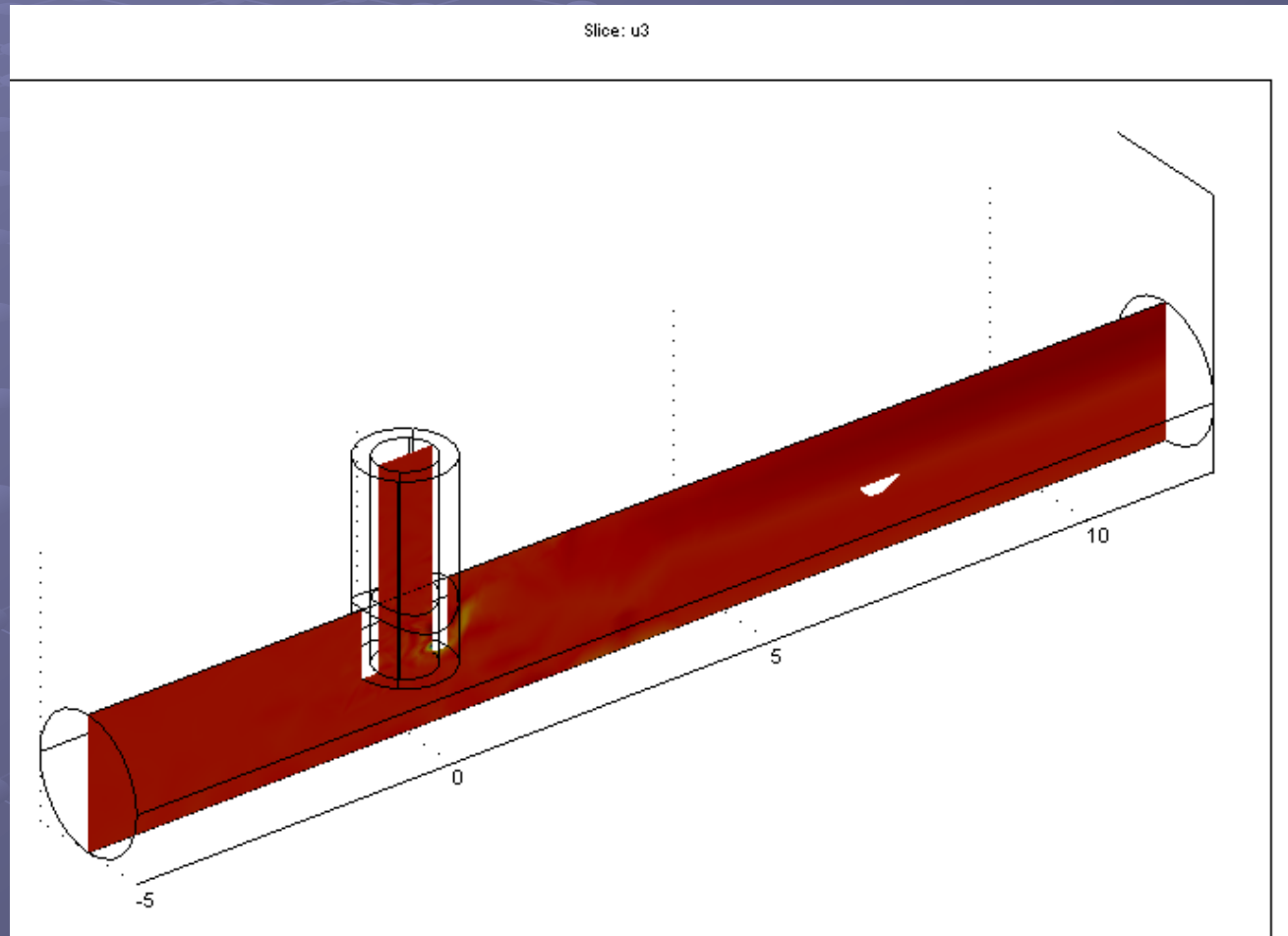
# Femlab results (varying Pe)



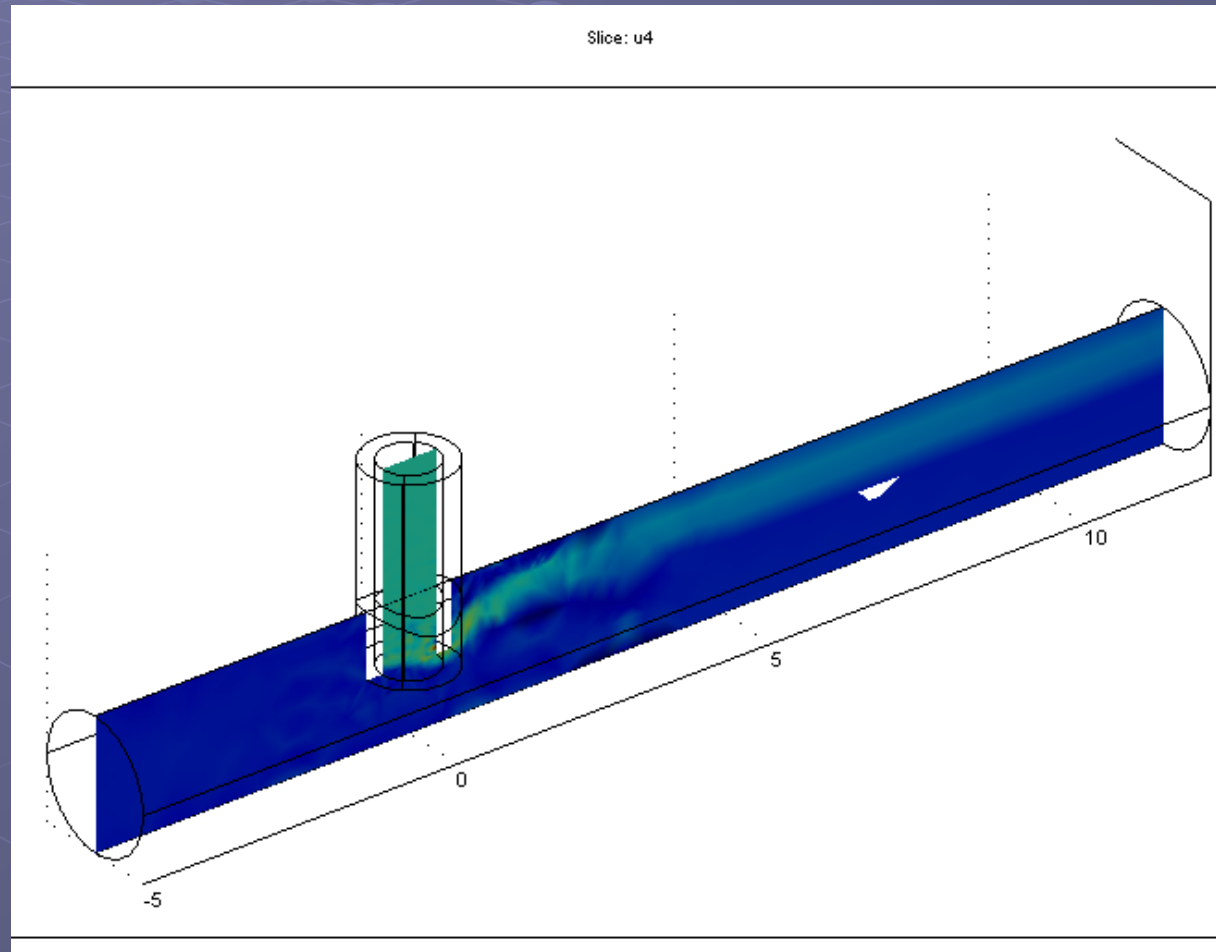
# Femlab results



# Femlab results

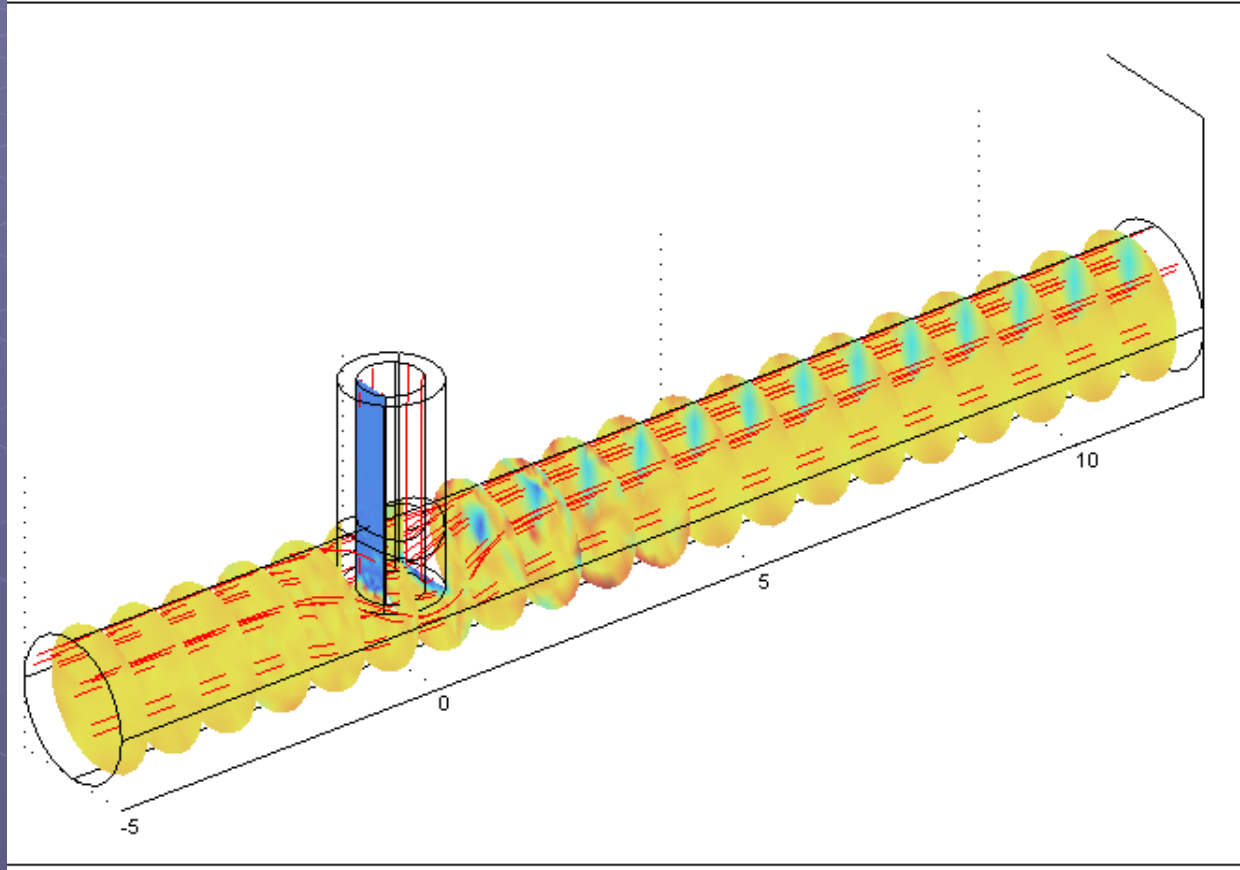


# Femlab results



# Femlab results

Slice: u1 Streamline: Velocity field



# Conclusion

- As rate constant increase conversion increase,
- As  $Pe$  increase conversion decrease, variance increase, avg concentration reagent increase, avg concentration product decrease

# About Femlab

- Solve all 5 equation separately in solve parameter.
- Then solve all four C-D equation together
- Try to increase it with smaller value if damping factor is to small but restart it with the value with results
- Activate inner boundary
- Deactivate the equation in subdomain within the cylinder.