In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import ipysheet as ips
import panel as pn
from scipy import stats
pn.extension('katex')
```

Tutorial 8

Tutorial problems on sorption and degradation

Homework problems on sorption and degradation

In [2]:
```
#Tutorial Problems
r4_1 = pn.pane.Markdown("""
# Tutorial Problems on Sorption and Degradation #

""",width = 900, style={'font-size': '13pt'})

r4_1
```

Out[2]:

Tutorial Problems on Sorption and Degradation

In [6]:
```
#Tutorial Problem 24
r5_1 = pn.pane.LaTeX(r"""

Tutorial Problem 24
<br><br>

A series of batch experiments were performed to quantify adsorption of Cr(VI) at bed soil of River Elbe
(solid density $\rho$ = 2.7 g/cm³, effective porosity $n_e = 30 \%$). For each experiment 10 g of bed soi
l was
equilibrated in 25 mL of water with initial Cr(VI) concentrations $C$ ranging from 50 to 250 mg/L (see ta
ble).
""",width = 600, style={'font-size': '13pt'})

r5_2 = pn.pane.LaTeX(r"""
a) Calculate the mass ratio $C_a$ of adsorbate vs. adsorbent for each batch experiment by employing the m
ass budget:

$$V_w \cdot C_0 = V_w \cdot C_{eq} + M_s\cdot C_a$$

with $V_w$ = water volume, $M_s$ = solid mass.<br>
<br>

b) Determine the distribution coefficient $K_d$ graphically by assuming that sorption of Cr(VI) can be de
scribed by a linear isotherm.
<br>
c) What is the retardation factor of Cr(VI) migrating through River Elbe bed soil? Briefly interpret your
result.

""",width = 600, style={'font-size': '13pt'})

r5_3 = pn.pane.LaTeX(r"""

$$C_a = \frac{V_w \cdot (C_0 - C_{eq})}{M_s}$$

""", style={'font-size': '13pt'})

d24_Co = np.array([50, 75, 100, 150, 200, 250])
d24_Ceq =  np.array([15, 28, 40, 61, 82, 104])

d24 = {"Co [mg/L]":d24_Co, "Ceq [mg/L]":d24_Ceq}
```

```
df24 = pd.DataFrame(d24)

spacer = pn.Spacer(width=50)

r5_4= pn.Column(r5_1, r5_2 )
r5_5= pn.Column(df24, r5_3 )
pn.Row(r5_4, spacer, r5_5)
```

Out[6]:

Tutorial Problem 24

A series of batch experiments were performed to quantify adsorption of Cr(VI) at bed soil of River Elbe (solid density ρ = 2.7 g/cm³, effective porosity $n_e = 30\%$). For each experiment 10 g of bed soil was equilibrated in 25 mL of water with initial Cr(VI) concentrations C ranging from 50 to 250 mg/L (see table).

a) Calculate the mass ratio C_a of adsorbate vs. adsorbent for each batch experiment by employing the mass budget:

$$V_w \cdot C_0 = V_w \cdot C_{eq} + M_s \cdot C_a$$

with V_w = water volume, M_s = solid mass.

b) Determine the distribution coefficient K_d graphically by assuming that sorption of Cr(VI) can be described by a linear isotherm.

c) What is the retardation factor of Cr(VI) migrating through River Elbe bed soil? Briefly interpret your result.

	Co [mg/L]	Ceq [mg/L]
0	50	15
1	75	28
2	100	40
3	150	61
4	200	82
5	250	104

$$C_a = \frac{V_w \cdot (C_0 - C_{eq})}{M_s}$$

In [4]:
```
# Solution of Problem 24 a

r5_6 = pn.pane.Markdown("""
## Solution Problem 24 a.
(**Check Lecture 09, Slides 11--13 for more information**)

""",width = 600, style={'font-size': '13pt'})

#Given
Vw = 25/1000 # L, volume of water in L
Ms = 10 # g, mass of Cr(IV)

# calculation
d24_Ca = Vw/Ms*(d24_Co-d24_Ceq) # Ca  = Vw/Ms* (Co-Ceq)

#output
d24_a = {"Co [mg/L]":d24_Co, "Ceq [mg/L]":d24_Ceq, "Ca [mg/g]":d24_Ca}
df24_a = pd.DataFrame(d24_a)
pn.Column(r5_6, df24_a)
```

Out[4]:

Solution Problem 24 a.

(**Check Lecture 09, Slides 11–13 for more information**)

	Co [mg/L]	Ceq [mg/L]	Ca [mg/g]
0	50	15	0.0875
1	75	28	0.1175
2	100	40	0.1500
3	150	61	0.2225
4	200	82	0.2950
5	250	104	0.3650

In [31]:
```
# Solution problem 24b
r5_7 = pn.pane.Markdown("""
### Solution Problem 24 b.
<br>
The linear isotherm is the regression line through the origin of the _C<sub>a</sub>_ vs._C<sub>eq</sub>_
 plot.
Its slope is the distribution coefficient _K<sub>d</sub>_<br><br>
***Here:***<br><br>
K<sub>d</sub> = 3.19E-03 L/ g<br><br>
K<sub>d</sub> = 3.19 cm<sup>3</sup>/ g
""",width = 400, style={'font-size': '13pt'})

# Linear fit
slope, intercept, r_value, p_value, std_err = stats.linregress(d24_Ceq, d24_Ca) # linear regression

#output
fig = plt.figure()
plt.plot(d24_Ceq, d24_Ca, 'o', label=' provided data');
pred = intercept + slope*d24_Ceq # fit line
plt.plot(d24_Ceq, pred, 'r', label='y={:.2E}x+{:.2E}'.format(slope,intercept)) ;
plt.xlabel(r"Equilibrium concentration,$C_{eq} $ (mg/L)"); plt.ylabel(r"Mass Ratio, $C_{a} $ (mg/L)");
plt.grid(); plt.legend(fontsize=11);  plt.text(20, 0.30,'$R^2 = %0.2f$' % r_value)
plt.close() # otherwise we have 2 figure
r5_8 = pn.pane.Matplotlib(fig, dpi=300)

pn.Row(r5_7, r5_8)
```

Out[31]:

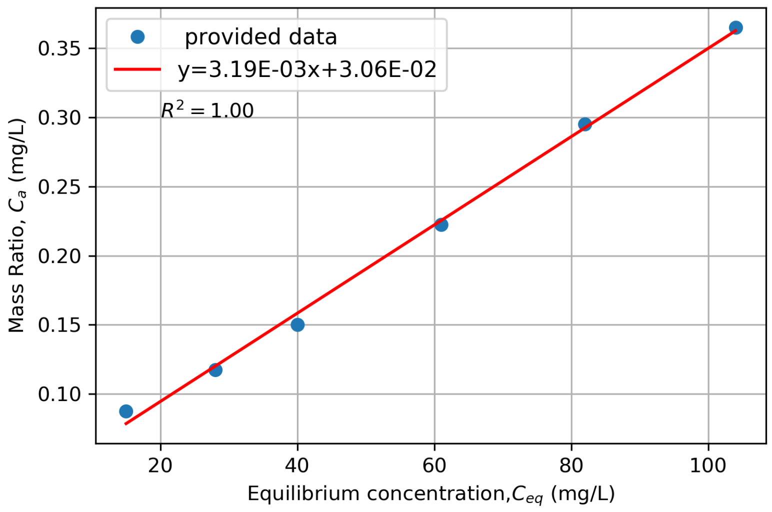
Solution Problem 24 b.

The linear isotherm is the regression line through the origin of the C_a vs.C_{eq} plot. Its slope is the distribution coefficient K_d

Here:

K_d = 3.19E-03 L/ g

K_d = 3.19 cm^3/ g



In [12]:
```
# Solution problem 24c
r5_9 = pn.pane.Markdown("""
### Solution Problem 15 c.
""",width = 400, style={'font-size': '13pt'})

r5_10 = pn.pane.LaTeX(r"""
$$ R = 1+ \frac{1-n_e}{n_e}\cdot \rho\cdot K_d $$
""",width = 400, style={'font-size': '13pt'})
pn.Column(r5_9, r5_10)
```

Out[12]:

Solution Problem 15 c.

$$R = 1 + \frac{1-n_e}{n_e} \cdot \rho \cdot K_d$$

In [13]:
```
#Given
rho = 2.7 # g/cm3 solid density
n_e = 0.30 # (), effective porosity
K_d = slope*1000 # cm^3/g, the slope of the plot, *1000 for unit conversion

# Calculate
R = 1 + ((1-n_e)/n_e)*rho*K_d

#output
print("The Retardation factor of the sample is: {0:1.2f}".format(R))
```

```
The Retardation factor of the sample is: 21.11
```

In [33]:
```
#Tutorial Problem 25
r6_1 = pn.pane.Markdown("""

## Tutorial Problem 25 ##
NaCl is used to conduct a conservative tracer test in a Darcy column (length: 85 cm, diameter: 7.5 cm).
The volumetric flow rate is 10 mL/min and the NaCl is continuously injected (concentration: 55 mg/L).
The table shows NaCl concentrations measured at the column outlet at different times.

""",width = 600, style={'font-size': '13pt'})

r6_2 = pn.pane.LaTeX(r"""
a) Normalise outlet concentration with injection concentration.<br>
b) Plot normalized concentration as a function of time.<br>
c) Determine graphically $t_{16}$, $t_{50}$, and $t_{84}$, where $t_x$ denotes the time when $x$% of the
injection concentration is reached at the column outlet.<br>
d) Determine effective porosity via $ n_e = \frac{Q\cdot t_{50}}{V}$ <br>
with $V$ = total volume of the column.<br>
e) Determine dispersivity via $\alpha = \frac{L}{8}\cdot \bigg(\frac{t_{84}-t_{16}}{t_{50}}\bigg)$

""",width = 600, style={'font-size': '13pt'})


d25_t = np.array([15, 30, 45, 60, 75, 90, 105, 120, 135, 150, 165, 180])
d25_C =  np.array([0, 0, 0, 2.5, 5.4, 10.6, 21.0, 29.1, 40.8, 51.7, 55.0, 55.0])

d25 = {"Time [min]":d25_t, "Conc. [mg/L]":d25_C}

df25 = pd.DataFrame(d25)

spacer = pn.Spacer(width=50)

r6_3= pn.Column(r6_1, r6_2 )
pn.Row(r6_3, spacer, df25)
```

Out[33]:

Tutorial Problem 25

NaCl is used to conduct a conservative tracer test in a Darcy column (length: 85 cm, diameter: 7.5 cm). The volumetric flow rate is 10 mL/min and the NaCl is continuously injected (concentration: 55 mg/L). The table shows NaCl concentrations measured at the column outlet at different times.

a) Normalise outlet concentration with injection concentration.
b) Plot normalized concentration as a function of time.
c) Determine graphically t_{16}, t_{50}, and t_{84}, where t_x denotes the time when x% of the injection concentration is reached at the column outlet.
d) Determine effective porosity via $n_e = \frac{Q \cdot t_{50}}{V}$
with V = total volume of the column.
e) Determine dispersivity via $\alpha = \frac{L}{8} \cdot \left(\frac{t_{84} - t_{16}}{t_{50}} \right)$

	Time [min]	Conc. [mg/L]
0	15	0.0
1	30	0.0
2	45	0.0
3	60	2.5
4	75	5.4
5	90	10.6
6	105	21.0
7	120	29.1
8	135	40.8
9	150	51.7
10	165	55.0
11	180	55.0

In [34]:
```
# solution 25a
r6_4 = pn.pane.Markdown("""
## Solution Problem 25 a.
(**Check Lecture 08, Slides 21--25 for more information**)

""",width = 600, style={'font-size': '13pt'})

#Given
C_m = 55 # mg/L, injected concentration

# calculation
d25_rc = d25_C/C_m # (-), Relative conc. Conc Out/Injected Con

#output
d25_a = d25 = {"Time [min]":d25_t, "Conc. [mg/L]":d25_C, "Rel. Conc [-]":d25_rc}
df25_a = pd.DataFrame(d25_a)
pn.Column(r6_4, df25_a)
```

Out[34]:

Solution Problem 25 a.

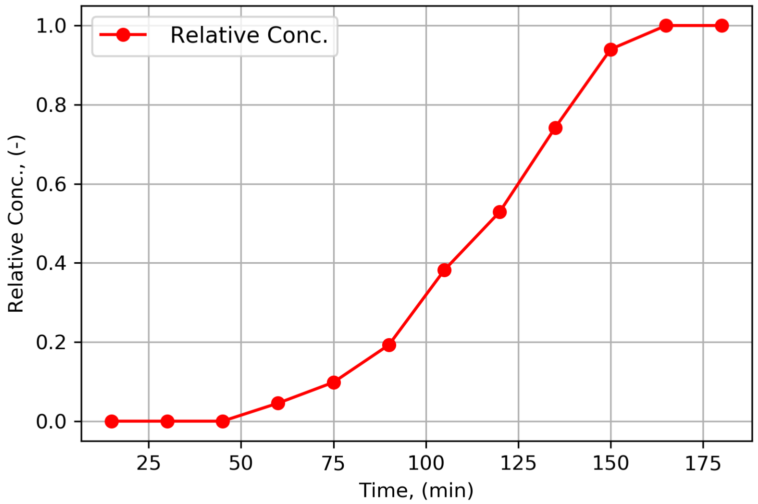
(Check Lecture 08, Slides 21–25 for more information)

	Time [min]	Conc. [mg/L]	Rel. Conc [-]
0	15	0.0	0.000000
1	30	0.0	0.000000
2	45	0.0	0.000000
3	60	2.5	0.045455
4	75	5.4	0.098182
5	90	10.6	0.192727
6	105	21.0	0.381818
7	120	29.1	0.529091
8	135	40.8	0.741818
9	150	51.7	0.940000
10	165	55.0	1.000000
11	180	55.0	1.000000

In [16]:
```
# Solution 25 b
r6_5 = pn.pane.Markdown("""  Solution Problem 25 b.
""",width = 300, style={'font-size': '13pt'})

# Plotting
fig = plt.figure()
plt.plot(d25_t, d25_rc, 'o-', color = "r", label=' Relative Conc.');
plt.xlabel(r"Time, (min)"); plt.ylabel(r"Relative Conc., (-)");
plt.grid(); plt.legend(fontsize=11);
plt.close() # otherwise we have 2 figure
r6_6 = pn.pane.Matplotlib(fig, dpi=300)

# Output
pn.Row(r6_5, r6_6)
```

Out[16]:

Solution Problem 25 b.



In [39]:
```
#Solution 25 c
r6_7 = pn.pane.Markdown("""Solution Problem 25 c. """,width = 300, style={'font-size': '13pt'})

fig = plt.figure()
plt.plot(d25_t, d25_rc, 'o-', color = "r", label=' Relative Conc.');
plt.xlabel(r"Time, (min)"); plt.ylabel(r"Relative Conc., (-)");
plt.grid(); plt.legend(fontsize=11);
plt.annotate(r't$_{16}$', xy=(82, 0.16),  xycoords='data',xytext=(0.0001, 0.16), textcoords='axes fractio
n',
             arrowprops=dict(facecolor='green', shrink=0.01),horizontalalignment='left', verticalalignmen
t='bottom',)
plt.annotate('', xy=(82, 0.0),  xycoords='data',xytext=(0.409, 0.16), textcoords='axes fraction',
             arrowprops=dict(facecolor='green', shrink=0.01),horizontalalignment='left', verticalalignmen
t='bottom',)
plt.annotate(r't$_{50}$', xy=(118, 0.5),  xycoords='data',xytext=(0.0001, 0.5), textcoords='axes fractio
n',
             arrowprops=dict(facecolor='green', shrink=0.01),horizontalalignment='left', verticalalignmen
t='bottom',)
plt.annotate('', xy=(118, 0.001),  xycoords='data',xytext=(0.61, 0.48), textcoords='axes fraction',
             arrowprops=dict(facecolor='green', shrink=0.01),horizontalalignment='left', verticalalignmen
t='bottom',)
plt.annotate(r't$_{84}$', xy=(145, 0.86),  xycoords='data',xytext=(0.0001, 0.81), textcoords='axes fracti
on',
             arrowprops=dict(facecolor='green', shrink=0.01),horizontalalignment='left', verticalalignmen
t='bottom',)
plt.annotate('', xy=(145, 0.001),  xycoords='data',xytext=(0.76, 0.80), textcoords='axes fraction',
             arrowprops=dict(facecolor='green', shrink=0.01),horizontalalignment='left', verticalalignmen
t='bottom',)
plt.close() # otherwise we have 2 figure
r6_8 = pn.pane.Matplotlib(fig, dpi=300)

r6_9 = pn.pane.LaTeX(r"""
From the figure:<br>
$t_{16}\approx 80$<br>
$t_{50}\approx 120$<br>
$t_{84}\approx 145$<br>

""",width = 300, style={'font-size': '13pt'})

r6_10 = pn.Column(r6_7, r6_9)
```

```
pn.Row(r6_10, r6_8)
```

Out[39]:

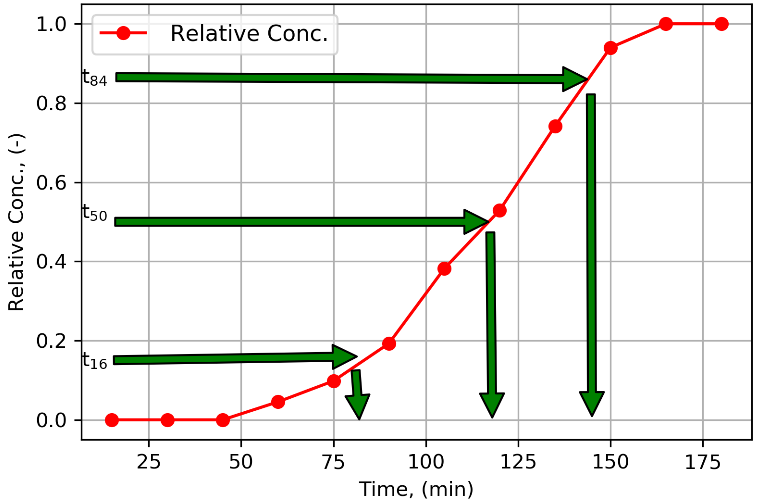
Solution Problem 25 c.

From the figure:

$t_{16} \approx 80$

$t_{50} \approx 120$

$t_{84} \approx 145$



In [41]:

```
#Solution 25 d

#Given
Q = 10 # mL/min, discharge in column
dc = 7.5 # cm, diameter of column
Lc = 85 # cm, length of column
t_50 = 120 # min, obtained from 17c

# Calculation
Vc = np.pi*(dc/2)**2*Lc # cm^3, Volume of column pi*d^2/4* h-
n_ef = Q*t_50/Vc # (-), effective porosity from given formula

#output
print("The effective porosity in the column is {0:1.2f}".format(n_ef))
```

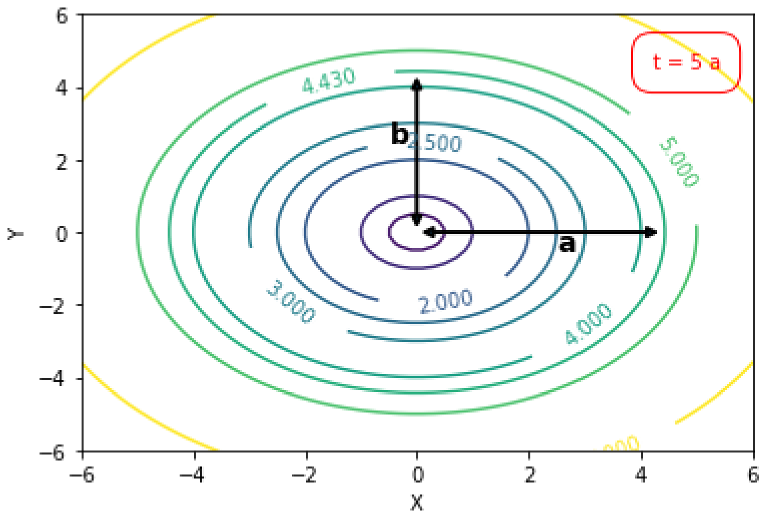
```
The effective porosity in the column is 0.32
```

In [40]:
```
#Solution 25 e

#Given
t_16 = 80 # min, obtained from 17c
t_84 = 145 # min, obtained from 17c
Lc = 85 # cm, length of column

# Calculation
alpha = Lc/8*((t_84-t_16)/t_50)**2

#output
print("The required dispersivity in the column is {0:1.2f}".format(alpha))
```

```
The required dispersivity in the column is 3.12
```

In [20]:
```
# contour plot code

import numpy as np
import matplotlib.pyplot as plt

x = np.linspace(-10.0, 10.0, 100)
y = np.linspace(-10.0, 10.0, 100)
X, Y = np.meshgrid(x, y)
Z = np.sqrt(np.square(X) + np.square(Y))

levels = [0.0, 0.5, 1.0, 2.0, 2.5, 3.0, 4.0, 4.43, 5, 7.0]
cp = plt.contour(X, Y, Z, levels)
plt.clabel(cp, inline=1, fontsize=10)
plt.xlabel('X');plt.ylabel('Y')
plt.xlim([-6, 6]); plt.ylim([-6, 6]);
plt.annotate("",xy=(0.0, 0.0), xycoords='data', xytext=(0.0, 4.4), textcoords='data',
arrowprops=dict(arrowstyle="<|-|>",lw=2,  connectionstyle="arc3"))
plt.annotate("",xy=(0.0, 0.0), xycoords='data', xytext=(4.4, 0), textcoords='data',
arrowprops=dict(arrowstyle="<|-|>", lw=2, connectionstyle="arc3"),)
plt.text(-0.5, 2.5, "b", fontweight="bold", fontsize= 14); plt.text(2.5, -0.5, "a", fontweight="bold", fo
ntsize= 14);
plt.text(4.2, 4.5, 't = 5 a', color='red', bbox=dict(facecolor='none', edgecolor='red', boxstyle='round,p
ad=1'))
```

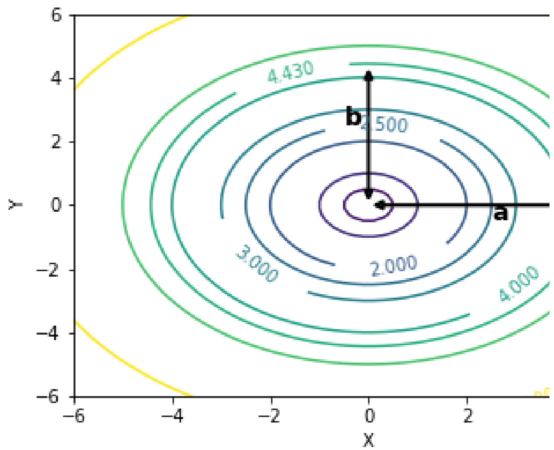
Out[20]: Text(4.2, 4.5, 't = 5 a')



In [21]:
```
#Problem 26

r7_1 = pn.pane.Markdown("""## Tutorial Problem 26 """,width = 600, style={'font-size': '13pt'})

r7_2 = pn.pane.LaTeX(r"""
A conservative tracer experiment was performed under following conditions:<br>

i) steady uniform flow in an aquifer with thickness $m = 10$ m and effective porosity $n_e = 0.2$<br>
ii) linear velocity: $v_x = 2\cdot 10^{-5}$ m/s, $v_y = 0$<br>
iii) dispersivities $\alpha_L = 0.5$ m, $\alpha_T = 0.2$ m<br>
iv) At $t = 0$, a tracer mass of $M = 985$ kg was injected at $(x_0, y_0) = (0, 250)$ m.<br>
v) The tracer is not subject to sorption or degradation, i.e., $R = 1$, $\lambda = 0$.
""",width = 600, style={'font-size': '13pt'})

r7_3 = pn.pane.LaTeX(r"""
<strong>Questions:</strong> <br>
a) Where is the centre of the tracer mass after a period of $t = 5$ a?
<br>
b) Where is the concentration isoline $C^\ast = 4.43$ mg/L at that time?
(Hint: Follow instructions given on next page to solve a) and b)).
.
""",width = 600, style={'font-size': '13pt'})

r7_4 = pn.pane.PNG("images/T05_3a.png", width=380)

r7_5 = pn.Column(r7_1, r7_2, r7_3)
pn.Row(r7_5, r7_4)
```

Out[21]:

Tutorial Problem 26



A conservative tracer experiment was performed under following conditions:
i) steady uniform flow in an aquifer with thickness $m = 10$ m and effective porosity $n_e = 0.2$
ii) linear velocity: $v_x = 2 \cdot 10^{-5}$ m/s, $v_y = 0$
iii) dispersivities $\alpha_L = 0.5$ m, $\alpha_T = 0.2$ m
iv) At $t = 0$, a tracer mass of $M = 985$ kg was injected at $(x_0, y_0) = (0, 250)$ m.
v) The tracer is not subject to sorption or degradation, i.e., $R = 1$, $\lambda = 0$.

Questions:

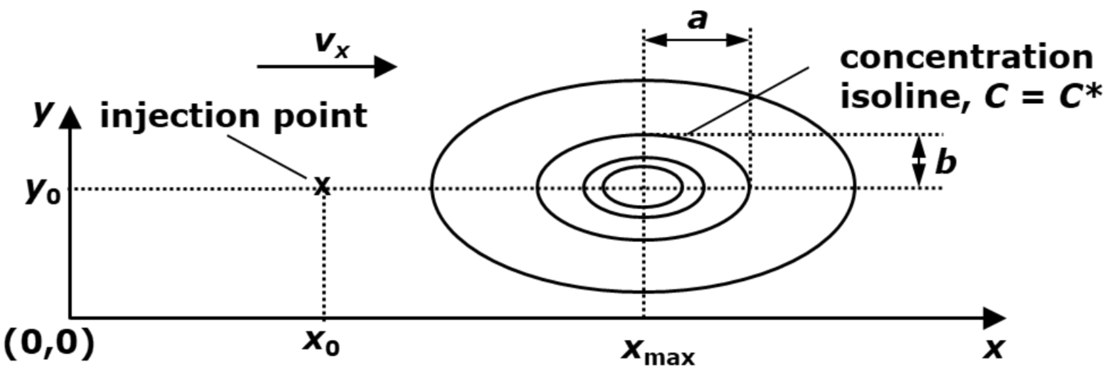
a) Where is the centre of the tracer mass after a period of $t = 5$ a?
b) Where is the concentration isoline $C^* = 4.43$ mg/L at that time? (Hint: Follow instructions given on next page to solve a) and b)). .

In [22]:
```
# Solution of Problem 26
r7_6 = pn.pane.Markdown("""
## Solution of Problem 26
(**Check Lecture 08, Slides 21--25 for more information**)
""",width = 800, style={'font-size': '13pt'})

r7_7 = pn.pane.PNG("images/T05_3b.png", width=600)

r7_8 = pn.pane.LaTeX(r"""
<br>
Concentration isolines are elliptic in the given scenario.
Four steps are to be performed to answer problems a) and b):<br>
<br>
<strong>Step 1:</strong> Find centre of ellipse given by $x_{max} = x_0 + v_x \cdot t/R$ and $y_{max} = y
_0$<br><br>
<strong>Step 2:</strong> Find peak concentration
$ C_{max} = \frac{M}{4\cdot \pi \cdot n_e \cdot m \sqrt{\alpha_L \cdot \alpha_T\cdot v_x \cdot t} }
\cdot e^{-\lambda\cdot t/R}$<br><br>
<strong>Step 3:</strong>: Calculate concentration ratio $f = C^\ast\times/C_{max}$<br><br>
<strong>Step 4:</strong> Determine lengths of semi-axes
$a = \sqrt{-4 \cdot \ln f \cdot \alpha_L \cdot v_x \cdot t/R}$ and
$b = \sqrt{\alpha_T/\alpha_L}\cdot a $

""",width = 800, style={'font-size': '13pt'})
pn.Column(r7_6, r7_7, r7_8)
```

Out[22]:

Solution of Problem 26

(**Check Lecture 08, Slides 21–25 for more information**)



Concentration isolines are elliptic in the given scenario. Four steps are to be performed to answer problems a) and b):

Step 1: Find centre of ellipse given by $x_{max} = x_0 + v_x \cdot t/R$ and $y_{max} = y_0$

Step 2: Find peak concentration $C_{max} = \frac{M}{4 \cdot pi \cdot n_e \cdot m \sqrt{\alpha_L \cdot \alpha_T \cdot v_x \cdot t}} \cdot e^{-\lambda \cdot t/R}$

Step 3:: Calculate concentration ratio $f = C^* \times /C_{max}$

Step 4: Determine lengths of semi-axes $a = \sqrt{-4 \cdot \ln f \cdot \alpha_L \cdot v_x \cdot t/R}$ and $b = \sqrt{\alpha_T/\alpha_L} \cdot a$

In [23]:
```
# Solution of Problem 26, STEP 1
#Given
x_o = 0 # m, starting point along x-direction
y_o = 250 # m, starting point along y-direction
v_x = 2*1e-5 # m/s Groundwater velocity
t = 5 # a, time in year
R = 1# (-), retardation factor

#calculate
t_s = t*365*24*3600 # s, time unit conversion
x_max = x_o + v_x*t_s/R
y_max = y_o

#output
print("The x_max is located at:{0:1.2f}".format(x_max), "m \n" )
print("The y_max is located at:{0:1.2f}".format(y_max), "m" )
```

```
The x_max is located at:3153.60 m

The y_max is located at:250.00 m
```

In [24]:
```
# Solution of Problem 26, STEP 2
# Given
M = 985 # kg, mass
n_ef = 0.2 # (-), effective porosity
m = 10 # m, aquifer thickness
a_L = 0.5 # m, longitudinal dispersivity
a_T = 0.2 # m, Transverse dispersivity
L_a = 0 #  (-), degradation rate, Lambda

# Compute
C_max = M/(4*np.pi* n_ef*m* np.sqrt(a_L*a_T)*v_x*t_s)*np.exp(-0*t_s/R)

print("The C_max is: {0:1.2e}".format( C_max), "Kg/m\u00b3 \n" )
print("The C_max is: {0:1.2f}".format(C_max*1000), "mg/L" )
```

```
The C_max is: 3.93e-02 Kg/m³

The C_max is: 39.30 mg/L
```

In [25]:

```python
# Solution of Problem 26, STEP 3 and Step 4

#Given
C_ast = 4.43 # mg/L concentration whose location is to be found
C_maxf = C_max*1000 # mg/L converting unit of C_max from Kg/m to mg/L

# Compute f
f = C_ast/C_maxf

# Solution Step 4

# compute a and b
a = np.sqrt(-4*np.log(f)*a_L*v_x*t_s/R)
b = np.sqrt(a_T/a_L)*a

#Output
print("The f is: {0:1.4f}".format(f) )
print("The a is: {0:1.2f}".format(a), "m")
print("The b is: {0:1.2f}".format(b), "m")
```

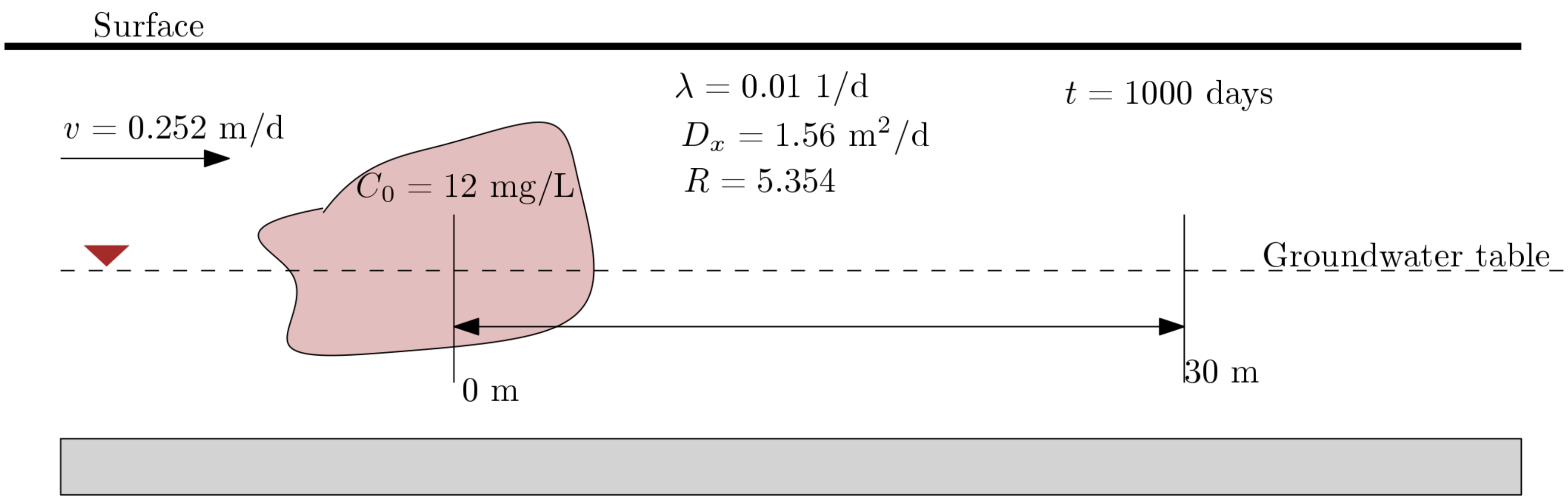
```
The f is: 0.1127
The a is: 117.33 m
The b is: 74.21 m
```

In [18]:
```
#Problem 27

r27_1 = pn.pane.Markdown("""## Tutorial Problem 27 """,width = 800, style={'font-size': '13pt'})

r27_2 = pn.pane.LaTeX(r"""
A contaminated site is to be evaluated for a potential spread of contaminat
from a source with an uniform concentration 12 mg/L (see figure below). The observation is to be
made at 30 m from the source for over 1000 days. The available informations are
the first order decay constant of the sediment is 0.01 1/d and soil retardation
coefficient is 5.354. The groundwater velocity in the aquifer is 0.252 m/d and
the longitudinal dispersion was computed to be 1.56 m$^2$/d.
""",width = 800, style={'font-size': '13pt'})

r27_4 = pn.pane.PNG("images/T08_TP27.png", width=800)


pn.Column(r27_1, r27_2, r27_4)
```

Out[18]:

Tutorial Problem 27

A contaminated site is to be evaluated for a potential spread of contaminat from a source with an uniform concentration 12 mg/L (see figure below). The observation is to be made at 30 m from the source for over 1000 days. The available informations are the first order decay constant of the sediment is 0.01 1/d and soil retardation coefficient is 5.354. The groundwater velocity in the aquifer is 0.252 m/d and the longitudinal dispersion was computed to be 1.56 m^2/d.



solution of Problem 27

The site is to be modeled using analytical solution provided in Wexler (1992). The provided solution for contaminant transport is $C(x,t)$:

$$C(x,t) = \frac{C_o}{2}\left[\exp\left(\frac{x}{2(D_x/R)}\left(\frac{v_x}{R}-\sqrt{\left(\frac{v_x}{R}\right)^2+4\lambda\frac{D_x}{R}}\right)\right)\cdot \mathrm{erfc}\left(\frac{x-t\sqrt{(v_x/R)^2+4\lambda(D_x/R)}}{2\sqrt{Dx/Rt}}\right)+\exp\left(\frac{x}{2(D_x/R)}\left(\frac{v_x}{R}+\sqrt{\left(\frac{v_x}{R}\right)^2+4\lambda\frac{D_x}{R}}\right)\right)\cdot \mathrm{erfc}\left(\frac{x+t\sqrt{(v_x/R)^2+4\lambda(D_x/R)}}{2\sqrt{Dx/Rt}}\right)\right]$$

we implement this solution to obtain the concentration at 30 m from the source for over 3 years time.

Wexler, E. 1992. *“Analytical Solutions for One-, Two-, and Three-Dimensional Solute Transport in Groundwater Systems with Uniform Flow.”* In Techniques of Water-Resources Investigations of the United States Geological Survey, 190. Book 3, Chapter B7.

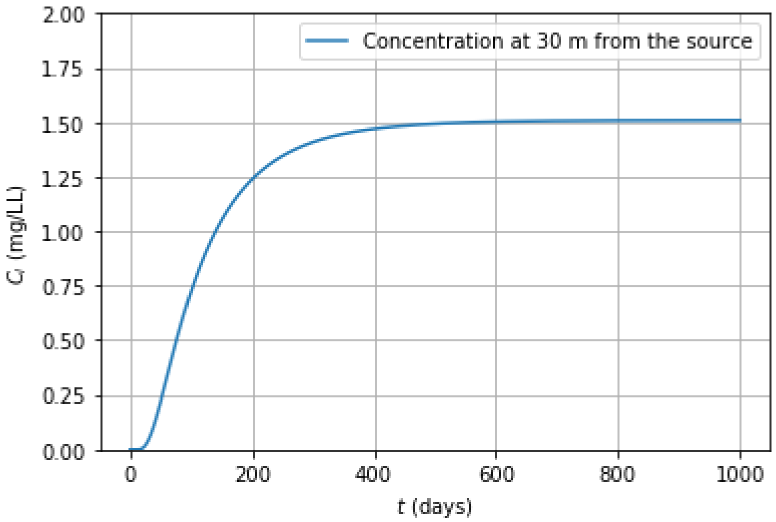
In [42]:

```
# Solution proble 27 continued
# INPUT

Dx = 7.56 #m^2/d disp coeff
vx = 0.252 # m/d gw velocity
R = 5.354 # [] retardation
Co = 12 # mg/L in concentration
x = 30 # m distance
ld = 0.01 # 1/d lambda
t = np.linspace(0, 1000, 1000)

# interim calculations

f1 = Dx/R
f2 = vx/R
f3 = np.sqrt(f2**2+ 4*ld*f1)

import scipy.special as sc # Required for getting erfc function

T1 = np.exp(x/(2*f1)*(f2-f3))        # first exp term
T2 = sc.erfc((x-t*f3)/(2*np.sqrt(t)*f1))     # first erfc term
T3 = np.exp(x/(2*f1)*(f2+f3))       # second exp term
T4 = sc.erfc((x+t*f3)/(2*np.sqrt(t)*f1))      # second erfc term
```

```
/home/prabhasyadav/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:21: RuntimeWarning: divide
by zero encountered in true_divide
/home/prabhasyadav/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:23: RuntimeWarning: divide
by zero encountered in true_divide
```

In [24]:
```
# solution P 27 contd.

# Calculation
C = Co/2*(T1*T2)+(T3*T4)

#plotting

plt.plot(t,C, label = "Concentration at 30 m from the source")
plt.grid()
plt.ylim((0,2))
plt.xlabel(r"$t$ (days)"); plt.ylabel(r"$C_i$ (mg/LL)")
plt.legend()
```

Out[24]: <matplotlib.legend.Legend at 0x7db72c17ae50>



HOME WORK PROBLEMS

Sorption and Degradation

There is no obligation to solve homework problems!

In [26]:

```
# Homework Problem 10
r8_1 = pn.pane.Markdown("""
## Homework Problem 10:


The same series of batch experiments as in tutorial problem 16 are considered. However, experimental find
ings are now to be evaluated
by assuming a Freundlich isotherm.

<br>
1. Plot decadic logarithm of mass ratio _C<sub>a</sub>_ vs. decadic logarithm of equilibrium concentratio
n _C<sub>eq</sub>_ in a diagram.

<br>
2. Determine the Freundlich coefficient _K<sub>Fr</sub>_ and the Freundlich exponent _n<sub>Fr</sub>_.

""",width = 900, style={'font-size': '13pt'})
r8_1
```

Out[26]:

Homework Problem 10:

The same series of batch experiments as in tutorial problem 16 are considered. However, experimental findings are now to be evaluated by assuming a Freundlich isotherm.

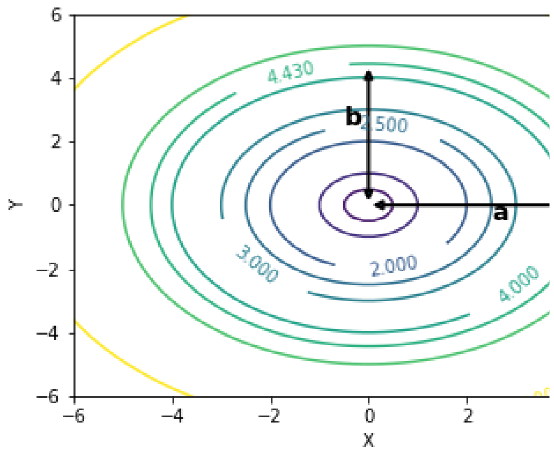
1. Plot decadic logarithm of mass ratio C_a vs. decadic logarithm of equilibrium concentration C_{eq} in a diagram.

2. Determine the Freundlich coefficient K_{Fr} and the Freundlich exponent n_{Fr}.

In [27]:
```
#Homework Problem 11

r9_1 = pn.pane.Markdown("""## Homework Problem 11 """,width = 600, style={'font-size': '13pt'})

r9_2 = pn.pane.LaTeX(r"""
A reactive tracer experiment was performed under following conditions:<br>

i) steady uniform flow in an aquifer with thickness $m = 10$ m and effective porosity $n_e = 0.2$<br>
ii) linear velocity: $v_x = 2\cdot 10^{-5}$ m/s, $v_y = 0$<br>
iii) dispersivities $\alpha_L = 0.5$ m, $\alpha_T = 0.2$ m<br>
iv) At $t = 0$, a tracer mass of $M = 985$ kg was injected at $(x_0, y_0) = (0, 250)$ m.<br>
v) The tracer is not subject to sorption or degradation, i.e., $R = 4.75$, $\lambda = 1\, a^{-1}$.
""",width = 600, style={'font-size': '13pt'})

r9_3 = pn.pane.LaTeX(r"""
<strong>Questions:</strong> <br>
a) Where is the centre of the tracer mass after a period of $t = 5$ a?
b) Where is the concentration isoline $C^\ast = 4.43$ mg/L at that time?
.
""",width = 600, style={'font-size': '13pt'})

r9_4 = pn.pane.PNG("images/T05_3a.png", width=380)

r9_5 = pn.Column(r9_1, r9_2, r9_3)
pn.Row(r9_5, r9_4)
```

Out[27]:

Homework Problem 11



A reactive tracer experiment was performed under following conditions:
i) steady uniform flow in an aquifer with thickness $m = 10$ m and effective porosity $n_e = 0.2$
ii) linear velocity: $v_x = 2 \cdot 10^{-5}$ m/s, $v_y = 0$
iii) dispersivities $\alpha_L = 0.5$ m, $\alpha_T = 0.2$ m
iv) At $t = 0$, a tracer mass of $M = 985$ kg was injected at $(x_0, y_0) = (0, 250)$ m.
v) The tracer is not subject to sorption or degradation, i.e., $R = 4.75$, $\lambda = 1\, a^{-1}$.

Questions:

a) Where is the centre of the tracer mass after a period of $t = 5$ a? b) Where is the concentration isoline $C^* = 4.43$ mg/L at that time? .