In [1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from BoreholeFlow import BhFlow
import quadprog as qp
from BoreholeFlow import PlotFigures
np.set_printoptions(precision=15)
from mpl_toolkits.axes_grid1 import make_axes_locatable, axes_size
```

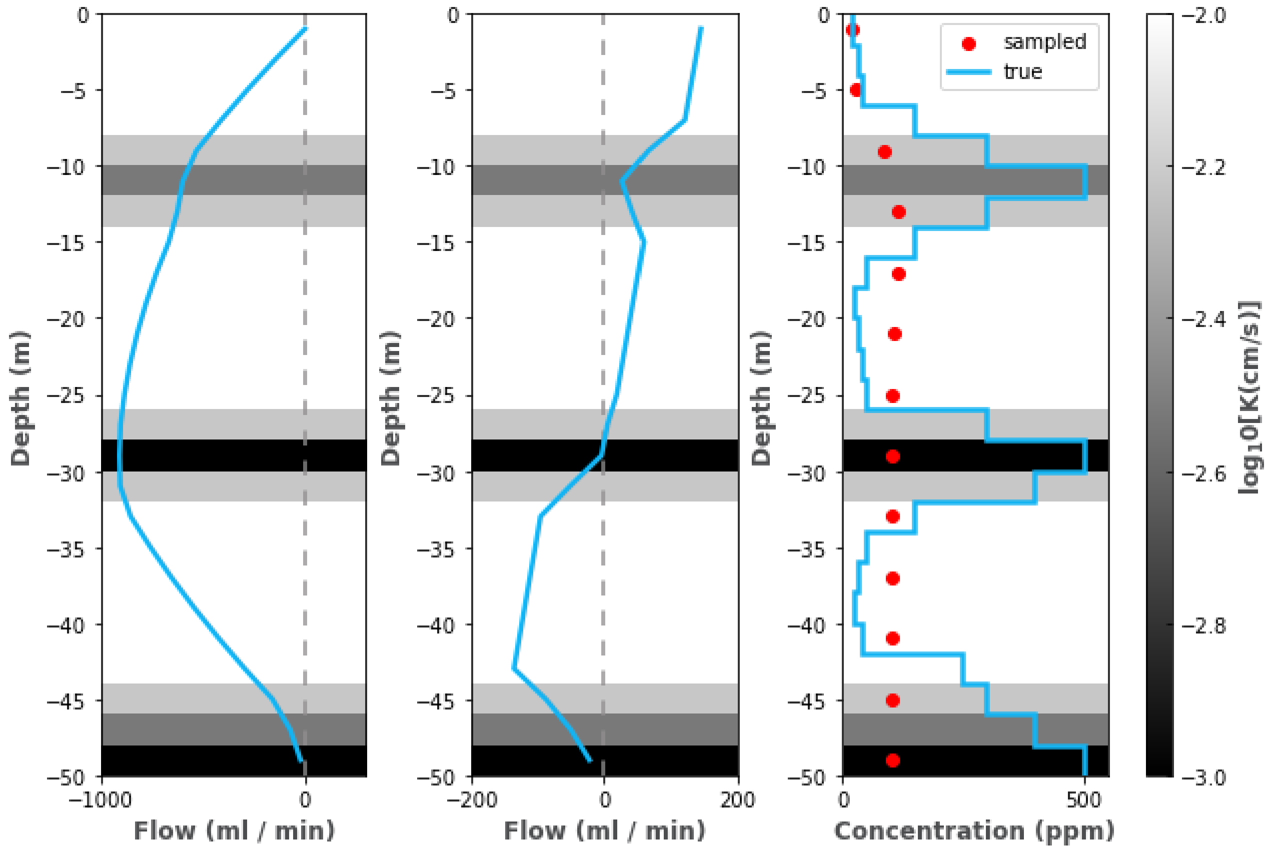
In [2]:
```
# Created by Joshua Thompson
# Last updated 09/02/2022

# -----------------------------------------------------
# EXAMPLE 3
# -----------------------------------------------------
alph = 1e-3
nskip = 2

R0 = 1000 # radius of influence for pumping (cm)
Rw = 20.32 / 2 # radius of well (cm)
dhtotal = 2.5 # drop in head from top to bottom of aquifer driving vertical flow

# Flow under ambient conditions
zpump = -100 * np.ones((1,1))
Qpump = np.zeros((1,1))
zobs = -100 * np.ones((1,1))
Qsampling = np.zeros((1,1))

nflows = len(Qpump)
zwellbot = -5000 # depth at bottom of screen

# Hydraulic conductivity (cm/s)
K = [1e-5, 3e-5, 6e-5, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 6e-5, 1e-5, 6e-5, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 6e-5,
K = np.array([i * 100 for i in K]).reshape(25, 1) # apply list comprehension for multiplying 100 by each element in lis

# True concentration in the aquifer (mg/cm^3)
C0 = np.array([500, 400, 300, 250, 40, 25, 30, 50, 150, 400, 500, 300, 50, 40, 30, 25, 50, 150, 300, 500, 300, 150, 40,
# C0 = C0.reshape((len(C0), 1))

# -----------------------------------------------------
# Instantiate the class
# -----------------------------------------------------
p = BhFlow(K, R0, Rw)
```

```
# Define number of layers based on the number of Ks
nlayers = p.NumberOfLayers()

# Create thickness of each wellbore interval
b = 200 * p.NlayersOnesArray(nlayers)
```

In [3]:
```
# Define layer head drops.
Keff = np.sum(b) / np.sum(b / K) # effective hydraulic conductivity

dh = Keff/K * b/np.sum(b) * dhtotal # head drops

h0 = p.NlayersZerosArray(nlayers) # Far field heads (in Aquifer)
h0[0] = dh[0] / 2 + 10000
for i in np.arange(1,nlayers):
    h0[i] = h0[i-1] + dh[i-1]/2 + dh[i]/2

ztop, zmid, zbot = p.Discretize(zwellbot, nlayers, b) # Discretize the well

# Run the borehole flow model
QbAmbient, QrAmbient, hAmbient, zmid, zbot, ztop = p.BoreholeFlowModel(nlayers, b, h0, zwellbot, ztop, zmid, zbot, zobs
```

In [4]:
```
zobs = np.arange(b[0] / 2, np.sum(b) - b[-1]/2 + 1, nskip * b[0]) + zwellbot
nobs = len(zobs)
Qsampling = 100 / 60

# Create empty list to store data
ctrueAll, cobsAll, gAll, zobsAll, zpumpAll, QpumpAll, QobsAll, QbAll, QrAll, hAll = p.MakeDataLists()

for i in range(len(zobs)):
    # Run flow model
    Qb, Qr, h, zmid, zbot, ztop= p.BoreholeFlowModel(nlayers, b, h0, zwellbot, ztop, zmid, zbot, zobs[i], zpump, Qpump,
    # Run transport model
    c, cobs, G = p.BoreholeTransportModel(nlayers, b, Qb, Qr, C0, ztop, zmid, zbot, zobs[i], zpump, Qpump, Qsampling)
    # Append data to empty lists
    ctrueAll, cobsAll, gAll, zobsAll, zpumpAll, QpumpAll, QobsAll, QbAll, QrAll, hAll = p.AppendData(c, cobs, G, zobs[i

# Convert list to array and transpose data
ctrueLF1, cobsLF1, GLF1, zobsLF1, zpumpLF1, QpumpLF1, QobsLF1, QbLF1, QrLF1, hLF1 = p.Convert2Arrays(zobs, nlayers, ctr
```

In [5]:
```
plot = PlotFigures()
plot.PlotFigure3(C0, K, QbAmbient, zmid, QrAmbient, cobsLF1, zobsLF1)
```



In [6]:
```
# ----------------------------------------------------
# EXPORTING FOR DATA VALIDATION
# ----------------------------------------------------
# path = r'C:\Users\thom675\OneDrive - PNNL\summer_internship_2022\borehole flow\Python\python_output'
# file_name1 = '\Python_Output_Fig3_QbLF1.txt'
# file_name2 = '\Python_Output_Fig3_QrLF1.txt'
# file_name3 = '\Python_Output_Fig3_ctrue.txt'
# file_name4 = '\Python_Output_Fig3_cobs.txt'

# np.savetxt(path + file_name1, QbLF1)
# np.savetxt(path + file_name2, QrLF1)
# np.savetxt(path + file_name3, ctrueLF1)
# np.savetxt(path + file_name4, cobsLF1)
```

In [1]:
```
import numpy as np
import pandas as pd
from scipy import signal
from scipy.signal import lsim
import matplotlib.pyplot as plt
from BoreholeFlow import BhFlow
from BoreholeFlow import PlotFigures
```

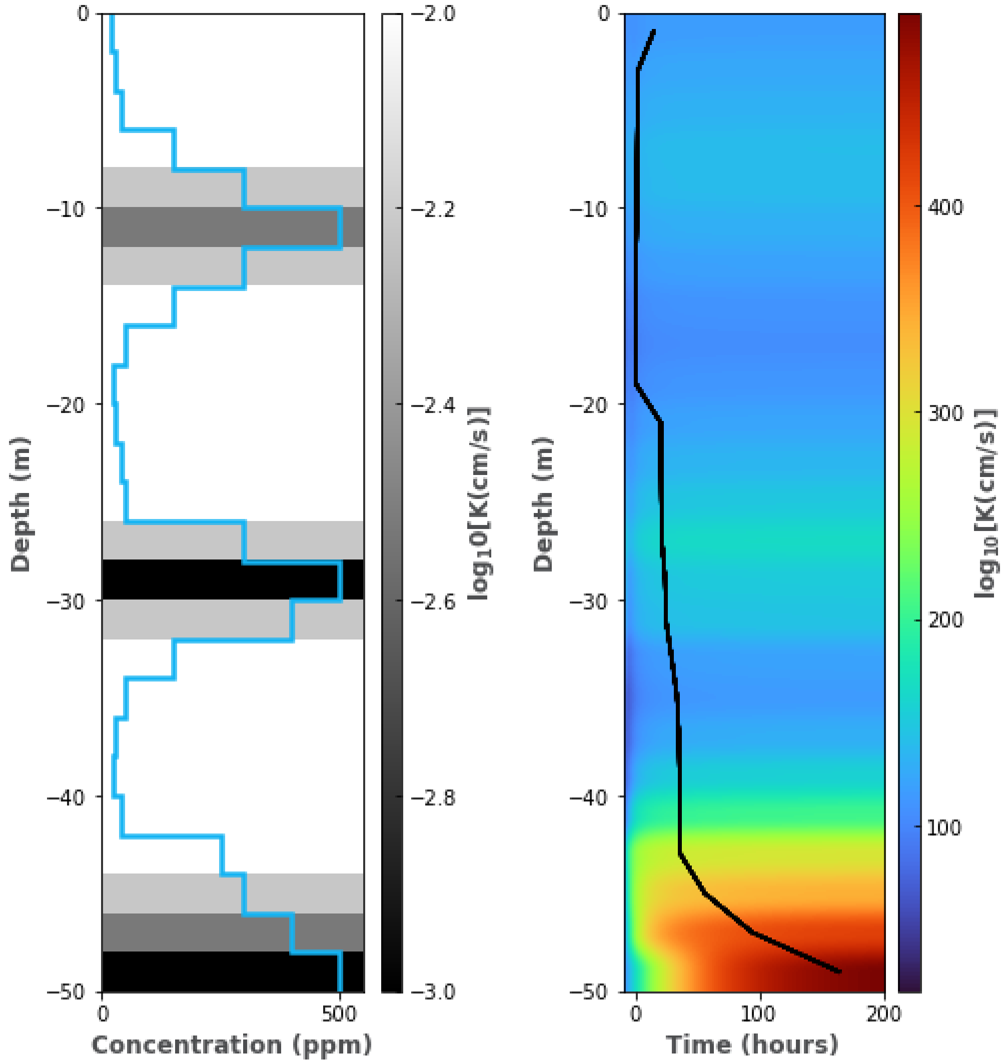
In [2]:
```
# Created by Joshua Thompson
# Last updated 09/02/2022
nskip = 1

R0 = 1000.0000
Rw = 20.32 / 2
dhtotal = 2.5

# Hydraulic conductivity (cm/s)
K = [1e-5, 3e-5, 6e-5, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 6e-5, 1e-5, 6e-5, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 6e-5,
K = np.array([i * 100 for i in K]).reshape(25, 1) # apply list comprehension for multiplying 100 by each element in lis

# True concentration in the aquifer (mg/cm^3)
C0 = np.array([500, 400, 300, 250, 40, 25, 30, 50, 150, 400, 500, 300, 50, 40, 30, 25, 50, 150, 300, 500, 300, 150, 40,

# -----------------------------------------------------
# Instantiate the class
# -----------------------------------------------------
p = BhFlow(K, R0, Rw)

# Define number of layers based on the number of Ks
nlayers = p.NumberOfLayers()

# Create thickness of each wellbore interval
b = 200 * p.NlayersOnesArray(nlayers)

zwellbot = -5000

# Define layer head drops.
Keff = np.sum(b) / np.sum(b / K) # effective hydraulic conductivity

dh = Keff/K * b/np.sum(b) * dhtotal # head drops

h0 = p.NlayersZerosArray(nlayers) # Far field heads (in Aquifer)
h0[0] = dh[0] / 2 + 10000
```

```
for i in np.arange(1,nlayers):
    h0[i] = h0[i-1] + dh[i-1]/2 + dh[i]/2

ztop, zmid, zbot = p.Discretize(zwellbot, nlayers, b) # Discretize the well

# ----------------------------------------------------
# ----------------------------------------------------
# Ambient flow
# ----------------------------------------------------
# ----------------------------------------------------
# Flow under ambient conditions
zpump = -100 * np.ones((1,1))
Qpump = np.zeros((1,1))
zobs = -100 * np.ones((1,1))
Qsampling = np.zeros((1,1))

# Create empty list to store data
ctrueAll, cobsAll, gAll, zobsAll, zpumpAll, QpumpAll, QobsAll, QbAll, QrAll, hAll = p.MakeDataLists()

for i in range(len(zobs)):
    # Run flow model
    Qb, Qr, h, zmid, zbot, ztop= p.BoreholeFlowModel(nlayers, b, h0, zwellbot, ztop, zmid, zbot, zobs[i], zpump, Qpump,
    # Run transport model
    c, cobs, G = p.BoreholeTransportModel(nlayers, b, Qb, Qr, C0, ztop, zmid, zbot, zobs[i], zpump, Qpump, Qsampling)
    # Append data to empty lists
    cssAmbient, cobsAmbient, gAmbient, zobsAmbient, zpumpAmbient, QpumpAmbient, QobsAmbient, QbAmbient, QrAmbient, hAmb

# ----------------------------------------------------
# ----------------------------------------------------
# Pump at 100cm depth at 8 L/min, approach to Steady State
# ----------------------------------------------------
# ----------------------------------------------------
Qpump = 8000 / 60
zpump = -100 * np.ones((1,1))
Qsampling = np.zeros((1,1))
zobs = np.arange(b[0] / 2, np.sum(b) - b[-1]/2 + 1, nskip * b[0]) + zwellbot
nobs = len(zobs)

tend = 24 * 60 * 60 * 10
t = np.linspace(0, tend, 1000)

ctrueAll, cobsAll, zobsAll, cssAll, tAll, QbAll, QrAll = p.MakeDataListsTransient()

for i in range(len(zobs)):
    Qb, Qr, h, zmid, zbot, ztop= p.BoreholeFlowModel(nlayers, b, h0, zwellbot, ztop, zmid, zbot, zobs[i], zpump, Qpump,
```

```
    c, css, cobs, tout = p.TransientTransportModel(t, nlayers, b, Qb, Qr, C0, cssAmbient[0], ztop, zmid, zbot, zobs[i],

    ctrueLF1, cobsLF1, zobsLF1, cssLF1, tLF1, QbLF1, QrLF1 = p.AppendDataTransient(c, cobs, zobs[i], css, t, Qb, Qr, ct
# Convert list to array
ctrueLF1, cobsLF1, zobsLF1, cssLF1, tLF1, QbLF1, QrLF1 = p.Convert2ArraysTransient(nlayers, zobs, t, ctrueAll, cobsAll,

cobsLF1T = cobsLF1.T

imin = []
for i in range(nobs):
    iset = np.argwhere(np.abs((cobsLF1T[:, i] - cssLF1[i]) / cssLF1[i]) < 0.05)[0]
    if iset.size> 0:
        imin.append(iset[0] + 1)
    else:
        imin.append(np.nan)
imin = np.asarray(imin)
tLF1T = tLF1.T
```

In [3]:

```
plot = PlotFigures()
plot.PlotFigure4(C0, K, zobs, cobsLF1, tLF1T, imin)
```



In [4]:
```
# ---------------------------------------------------
# EXPORTING FOR DATA VALIDATION
# ---------------------------------------------------
# path = r'C:\Users\thom675\OneDrive - PNNL\summer_internship_2022\borehole flow\Python\python_output'
# file_name = '\Python_Output_Fig4_CobsLF1.txt'

# np.savetxt(path + file_name, cobsLF1)
```

In [1]:
```
import numpy as np
from scipy import optimize
import pandas as pd
import matplotlib.pyplot as plt
from BoreholeFlow import BhFlow
from BoreholeFlow import invertBHconc
from BoreholeFlow import PlotFigures
import quadprog as qp
np.set_printoptions(precision=15)
```

In [2]:
```
# Created by Joshua Thompson
# Last updated 09/02/2022

path2randvector =  r"..\Input_Data\randvector.txt"
randvector = np.asarray(pd.read_csv(path2randvector, header = None))

alphmax = 1 #Upper bound for alpha
alph = 1e-3
concerr = 5
nskip = 2

R0 = 1000.0000
Rw = 20.32 / 2
dhtotal = 2.5

Qsampling = 100 / 60
zwellbot = -5000

# Hydraulic conductivity (cm/s)
K = [1e-5, 3e-5, 6e-5, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 6e-5, 1e-5, 6e-5, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 1e-4, 6e-5,
K = np.array([i * 100 for i in K]).reshape(25, 1) # apply list comprehension for multiplying 100 by each element in lis

# True concentration in the aquifer (mg/cm^3)
C0 = np.array([500, 400, 300, 250, 40, 25, 30, 50, 150, 400, 500, 300, 50, 40, 30, 25, 50, 150, 300, 500, 300, 150, 40,

# -----------------------------------------------------
# Instantiate the class
# -----------------------------------------------------
p = BhFlow(K, R0, Rw)

# Define number of layers based on the number of Ks
nlayers = p.NumberOfLayers()
```

```
# Create thickness of each wellbore interval
b = 200 * p.NlayersOnesArray(nlayers)

zobs = np.arange(b[0] / 2, np.sum(b) - b[-1]/2 + 1, nskip * b[0]) + zwellbot
nobs = len(zobs)

X = p.NlayersOnesArray(nlayers)

# Define layer head drops.
Keff = np.sum(b) / np.sum(b / K) # effective hydraulic conductivity

dh = Keff/K * b/np.sum(b) * dhtotal # head drops

h0 = p.NlayersZerosArray(nlayers) # Far field heads (in Aquifer)
h0[0] = dh[0] / 2 + 10000
for i in np.arange(1,nlayers):
    h0[i] = h0[i-1] + dh[i-1]/2 + dh[i]/2

ztop, zmid, zbot = p.Discretize(zwellbot, nlayers, b) # Discretize the well

# -----------------------------------------------------
# -----------------------------------------------------
# L-F dataset with no other pumping (Qpump=0)
# -----------------------------------------------------
# -----------------------------------------------------
zpump = -100 *np.ones((1,1))
Qsampling = 100 / 60
Qpump = np.zeros((1,1))

# Create empty list to store data
ctrueAll, cobsAll, gAll, zobsAll, zpumpAll, QpumpAll, QobsAll, QbAll, QrAll, hAll = p.MakeDataLists()

for i in range(len(zobs)):
    # Run flow model
    Qb, Qr, h, zmid, zbot, ztop= p.BoreholeFlowModel(nlayers, b, h0, zwellbot, ztop, zmid, zbot, zobs[i], zpump, Qpump,
    # Run transport model
    c, cobs, G = p.BoreholeTransportModel(nlayers, b, Qb, Qr, C0, ztop, zmid, zbot, zobs[i], zpump, Qpump, Qsampling)
    # Append data to empty lists
    ctrueLF1, cobsLF1, gLF1, zobsLF1, zpumpLF1, QpumpLF1, QobsLF1, QbLF1, QrLF1, hLF1 = p.AppendData(c, cobs, G, zobs[i
# Convert list to array and transpose data
ctrueLF1, cobsLF1, gLF1, zobsLF1, zpumpLF1, QpumpLF1, QobsLF1, QbLF1, QrLF1, hLF1 = p.Convert2Arrays(zobs, nlayers, ctr

cobsLF1 = cobsLF1 + randvector * concerr
s = invertBHconc(nlayers, gLF1, X, cobsLF1, concerr, alphmax, alph)
c0estLF1, rmsLF1, RLF1 = s.InvertData()
```

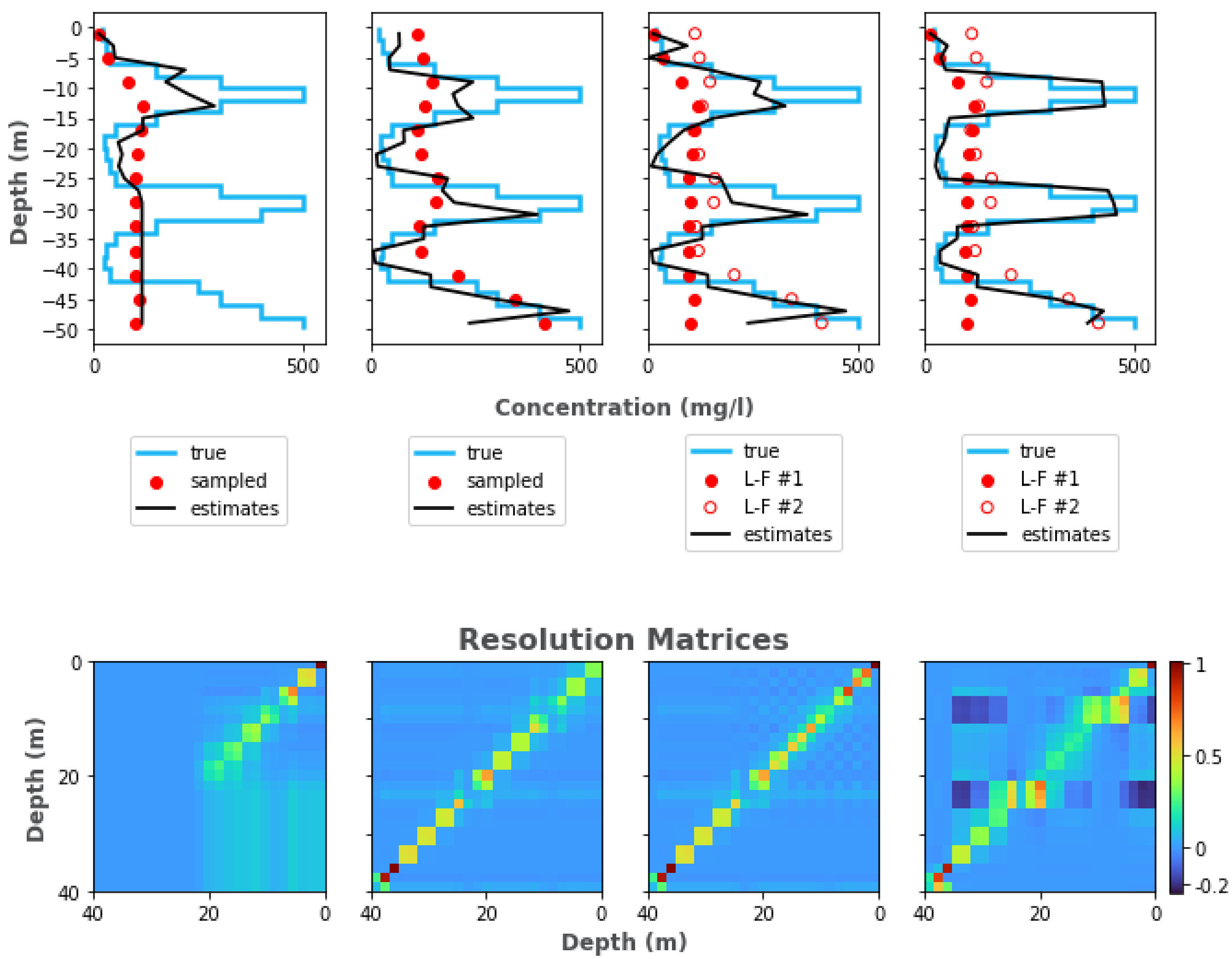
```
# ----------------------------------------------------
# ----------------------------------------------------
# L-F dataset with pumping (Qpump=8 L/min)
# ----------------------------------------------------
# ----------------------------------------------------
Qpump = 8000 / 60
Qsampling = 100/ 60
path2randvector2 = r"..\Input_Data\randvector2.txt"

randvector2 = np.asarray(pd.read_csv(path2randvector2, header = None))

# Create empty list to store data
ctrueAll, cobsAll, gAll, zobsAll, zpumpAll, QpumpAll, QobsAll, QbAll, QrAll, hAll = p.MakeDataLists()

for i in range(len(zobs)):
    # Run flow model
    Qb, Qr, h, zmid, zbot, ztop = p.BoreholeFlowModel(nlayers, b, h0, zwellbot, ztop, zmid, zbot, zobs[i], zpump, Qpump

#     Run transport model
    c, cobs, G = p.BoreholeTransportModel(nlayers, b, Qb, Qr, C0, ztop, zmid, zbot, zobs[i], zpump, Qpump, Qsampling)
#     Append data to empty lists
    ctrueLF2, cobsLF2, gLF2, zobsLF2, zpumpLF2, QpumpLF2, QobsLF2, QbLF2, QrLF2, hLF2 = p.AppendData(c, cobs, G, zobs[i

# Convert list to array and transpose data
ctrueLF2, cobsLF2, gLF2, zobsLF2, zpumpLF2, QpumpLF2, QobsLF2, QbLF2, QrLF2, hLF2 = p.Convert2Arrays(zobs, nlayers, ctr

cobsLF2 = cobsLF2 + randvector2 * concerr

s = invertBHconc(nlayers, gLF2, X, cobsLF2, concerr, alphmax, alph)
c0estLF2, rmsLF2, RLF2 = s.InvertData()

# ----------------------------------------------------
# ----------------------------------------------------
# Combined Dataset
# ----------------------------------------------------
# ----------------------------------------------------
ctrueCombine, cobsCombine, gCombine, zobsCombine, zpumpCombine, QpumpCombine, QobsCombine, QbCombine, QrCombine, hCombi
s = invertBHconc(nlayers, gCombine, X, cobsCombine, concerr, alphmax, alph)
c0estCombine, rmsCombine, RCombine = s.InvertData()

# ----------------------------------------------------
# ----------------------------------------------------
# # Consider non-uniform zonation (4 zones)
# ----------------------------------------------------
```

```
# -------------------------------------------------------
path2XZone = r"..\Input_Data\XZone.txt"
XZone = np.asarray(pd.read_csv(path2XZone, header = None, sep = '\s+'))
s = invertBHconc(nlayers, gCombine, XZone, cobsCombine, concerr, alphmax, alph)
c0estComX, rmsComX, RComX = s.InvertData()
```

```
negative concentrationm estimates produced; switching to quadratic programming -1.464335380142245
```

In [3]:

```
plot = PlotFigures()
plot.PlotFigure5(C0, cobsLF1, zobsLF1, c0estLF1, cobsLF2, zobsLF2, c0estLF2, c0estCombine[0], c0estComX, zmid, RLF1, RL
```



In [4]:

```
# -------------------------------------------------------
```

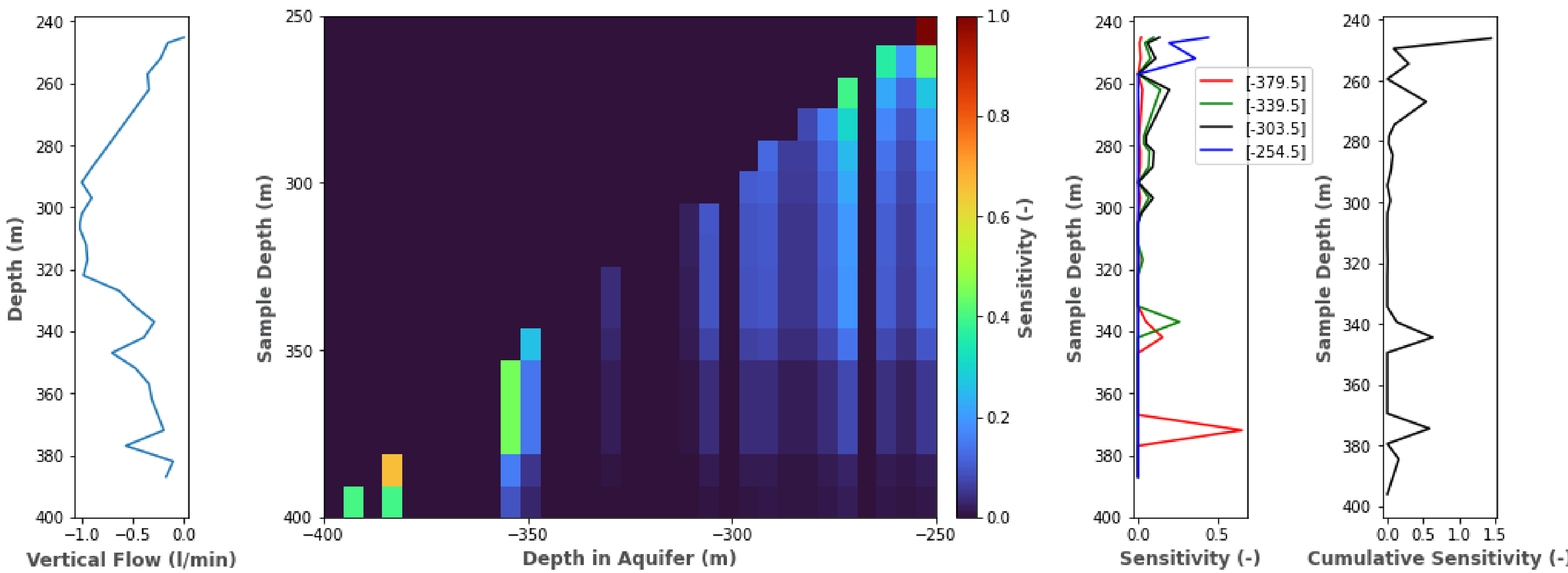
```
# EXPORTING FOR DATA VALIDATION
# ---------------------------------------------------
# path = r'C:\Users\thom675\OneDrive - PNNL\summer_internship_2022\borehole flow\QA\BoreholeFlow_Analysis\Output_Valida
# file_name1 = '\Python_Output_Fig5_c0estLF2.txt'
# file_name2 = '\Python_Output_Fig5_c0estCombine.txt'
# file_name3 = '\Python_Output_Fig5_c0estComX.txt'
# file_name4 = '\Python_Output_Fig5_RLF1.txt'
# file_name5 = '\Python_Output_Fig5_RLF2.txt'
# file_name6 = '\Python_Output_Fig5_RCombine.txt'
# file_name7 = '\Python_Output_Fig5_RComX.txt'


# np.savetxt(path + file_name1, c0estLF2)
# np.savetxt(path + file_name2, c0estCombine[0])
# np.savetxt(path + file_name3, c0estComX)
# np.savetxt(path + file_name4, RLF1)
# np.savetxt(path + file_name5, RLF2)
# np.savetxt(path + file_name6, RCombine)
# np.savetxt(path + file_name7, RComX)
```

In [1]:
```
import numpy as np
from scipy import optimize
import pandas as pd
import matplotlib.pyplot as plt
from BoreholeFlow import BhFlow
from BoreholeFlow import PlotFigures
import quadprog as qp
np.set_printoptions(precision=15)
```

In [2]:
```
# Created by Joshua Thompson
# Last updated 09/02/2022
Rw = 20.32 / 2
R0 = 1000

path_well_299_W15_225 = r"..\Input_Data\well_299_W15_225.txt"
flowlog = pd.read_csv(path_well_299_W15_225, header = None, sep = '\s+')

ztop = np.asarray(-flowlog.iloc[:, 0]).reshape(31, 1)
zbot = np.asarray(-flowlog.iloc[:, 1]).reshape(31, 1)
Qr = np.asarray(flowlog.iloc[:, 2]).reshape(31, 1)
Qb = np.asarray(flowlog.iloc[:, 3]).reshape(31, 1)

zwellbot = -np.min(zbot)
nlayers = len(Qb)

b = ztop - zbot

zmid = []
for i in range(len(ztop)):
    zm = np.mean((ztop[i], zbot[i]), dtype=np.float64)
    zmid.append(zm)
zmid = np.asarray(zmid)

Qerror = np.sum(Qr)
if(Qerror> 1e-5):
    print('borehole flows do not balance')

nskip = 2

Qsampling = np.zeros((1,1))
zpump = zmid[0]
Qpump = np.zeros((1,1))
zobs = np.asarray(zmid[0:31:nskip]).reshape(16, 1)
```

```
C0 = np.ones((nlayers, 1))

p = BhFlow(np.zeros((1,1)), R0, Rw)

# Create empty list to store data
ctrueAll, cobsAll, gAll, zobsAll, zpumpAll, QpumpAll, QobsAll, QbAll, QrAll, hAll = p.MakeDataLists()

for i in range(len(zobs)):
 # Run transport model
    c, cobs, G = p.BoreholeTransportModel(nlayers, b, Qb, Qr, C0, ztop, zmid, zbot, zobs[i], zpump, Qpump, Qsampling)
    # Append data to empty lists
    gAll.append(G)
gAll = np.asarray(gAll)
gAll = gAll.reshape(16, 31)
```

In [3]:
```
plot = PlotFigures()
plot.PlotFigure6(Qb, zobs, zmid, ztop, gAll)
```



In [4]:
```
# ----------------------------------------------------
# EXPORTING FOR DATA VALIDATION
# ----------------------------------------------------
# path = r'C:\Users\thom675\OneDrive - PNNL\summer_internship_2022\borehole flow\Python\python_output'
# file_name = '\Python_Output_Fig6_Gmatrix.txt'
```

```
# np.savetxt(path + file_name, gAll)
```