

NUEN 647
Uncertainty Quantification for Nuclear Engineering
Assignment 1

Due on Tuesday, October 4, 2016

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Complete the exercises in the Chapter 2 notes. Be sure to include discussion of results where appropriate. You may use any tools that are appropriate to solving the problem.

Problem 1

Listing 1 shows a Perl script.

Listing 1: Sample Perl Script With Highlighting

```
#!/usr/bin/perl

use strict;
use warnings;

5  for (1..99) { print $_." Luftballons\n"; }

# This is a commented line

10 my $string = "Hello World!";

    print $string."\n\n";

$string =~ s/Hello/Goodbye/;

15  print $string."\n\n";

    test();

20  exit;

sub test { print "All good.\n"; }
```

Listing 2: Sample python script no .py

```
#!/usr/bin/env python3

"""
Chem Calculations
5  """

__author__      = "Paul Mendoza"
__copyright__   = "Copyright 2016, Planet Earth"
__credits__     = ["Sunil Chirayath",
10  "Charles Folden",
    "Jeremy Conlin"]
__license__     = "GPL"
__version__     = "1.0.1"
__maintainer__  = "Paul Mendoza"
15  __email__     = "paul.m.mendoza@gmail.com"
    __status__   = "Production"

#####
##### Import packages #####
```

```

20 #####

import os.path
import pandas as pd
import numpy as np
25 import matplotlib.pyplot as plt
import datetime
from uncertainties import ufloat
from uncertainties.umath import *
from uncertainties import unumpy as unp
30 import re
import time
start_time = time.time()

import Functions as fun
35

#####
##### Examples of Calculations #####
#####

40 #####
##### Atom Fraction to Mass Fraction #####
##### and vice versa #####
#####

45 string='92235 0.285714286 0 92238 0.714285714 0'
MasstoAtom=True
Mass,Zaid=fun.StringToMass(string)
stringCalculated=fun.ConvertFractions(string,Mass,MasstoAtom,Zaid)
50

# if MasstoAtom:
#     print("Mass Fractions:")
#     print(string)
#     print("Atom Fractions:")
55 #     print(stringCalculated)
# else:
#     print("Mass Fractions:")
#     print(stringCalculated)
#     print("Atom Fractions:")
60 #     print(string)

#####
##### Calculate grams per mol of #####
##### a chemical formula #####
65 #####

#Make sure your chemical form has no repeats
#And no parentheses
ChemicalFormula='HNO_3'
70 ChemicalFormulaError=[0,0,0,0,0,0] #+/- error in integers of
                                     #chemical formula
ChemicalFormula=ChemicalFormula+" "

```

```

List=fun.ChemList (ChemicalFormula)

75 #Enter Modifications:
#1. Each element should be a single item in the list
#2. Format: zaid atomfraction+/-error zaid atomfraction+/-error
# or : zaid atomfraction error zaid atomfraction
Modifications=['92235 0.2883155436+/-0.0000000024 92238 0.7116844564+/-0.0000000024',stringCalcu

80
df = pd.read_csv('../Data/AtomicWeights.csv')

ModMass,ModSymbols,AtomFractions=fun.FormatMods (Modifications,df)
85 MolarMass=fun.DetermineMolarMass (List,df,
                                     ModSymbols,ModMass,
                                     AtomFractions,ChemicalFormulaError)

# print (MolarMass)

90
#####
##### Calculate Molality from #####
##### Wt % #####
#####

95
gramsOmol=MolarMass
WtConcentration=ufloat (69,0.1)
Molality=1000/(gramsOmol*(100/WtConcentration-1))

100
#####
##### Convert molality/molarity #####
#####

MolarityToMolality=True

105
gramsOmol=MolarMass

#Density in grams per cc or grams per ml
dfDen=pd.read_csv('../Data/Nitric_Acid.csv')

110
Temperature=ufloat (20,3) #Same degrees as dfDen!!!

Molality=Molality
Molarity=ufloat (15.43,0.06)

115
if MolarityToMolality:
    Molality=fun.ConvertMol (MolarityToMolality,Molarity,
                             gramsOmol,dfDen,Temperature)
else:
120    Molarity=fun.ConvertMol (MolarityToMolality,Molality,
                             gramsOmol,dfDen,Temperature)

#print ("Molarity = "+str(Molarity))
125 #print ("Molality = "+str(Molality))

```

```

#####
##### Calculate New Concentration #####
130 #####

Vol1=1
Vol2=1

135 gramsOmol=gramsOmol

m1=Molality
m2=Molality*.25

140 Temperature=ufloat(20,3)

dfDen=pd.read_csv('../Data/Nitric_Acid.csv')

145 m3,p3,Vol3,Wt,M3=fun.NewConcentration(m1,m2,gramsOmol,
                                         Temperature,dfDen,
                                         Vol1,Vol2)

M1=fun.ConvertMol(False,m1,gramsOmol,dfDen,Temperature)
M2=fun.ConvertMol(False,m2,gramsOmol,dfDen,Temperature)
150

##### Time To execute #####

print("--- %s seconds ---" % (time.time() - start_time))

```

Listing 3: Sample python script no .py

```

#!/usr/bin/env python3

"""
FractionAM converts atom fractions to mass fractions
5 and mass fractions to atom fractions. Input is a
single string with MCNP style fractions.
"""

__author__      = "Paul Mendoza"
10 __copyright__  = "Copyright 2016, Planet Earth"
__credits__     = ["Sunil Chirayath",
                  "Charles Folden",
                  "Jeremy Conlin"]

__license__     = "GPL"
15 __version__   = "1.0.1"
__maintainer__  = "Paul Mendoza"
__email__       = "paul.m.mendoza@gmail.com"
__status__      = "Production"

20 #####
##### Import packages #####
#####

```

```

import os.path
25 import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import datetime
from uncertainties import ufloat
30 from uncertainties.umath import *
from uncertainties import unumpy as unp
import re

#####
35 ##### Functions #####
#####

def ReturnUfloat(string):
    """
40     string has format      238.023249814(23)
                        or format  [15.99903-15.99977]
                        or format  235.04+/-0.0000019

    Returns a uncertain number so python can do calculations
45     """
    if "(" in string:
        Number=str(string.split('(')[0])
        LastErrorNumber=str(string.split("(")[1].replace(")", ""))
        NumberOfZeros=len(Number.split(".")[1])-len(LastErrorNumber)
50         Error="0."
        for i in range(0,NumberOfZeros):
            Error=Error+"0"
        Error=Error+LastErrorNumber
    elif "[" in string:
55         FirstNum=float(string.split('-')[0].replace("[", ''))
        SecondNum=float(string.split('-')[1].replace(']', ''))
        Number=str((FirstNum+SecondNum)/2)
        Error=str(float(Number)-FirstNum)
    elif "+/-" in string:
60         Number=string.split("+/-")[0]
        Error=string.split("+/-")[1]

    return(ufloat(float(Number),float(Error)))

65 def FindAtomicMass(df,proton,Isotope):
    """
    This function will take in a dataset 'df' look through the
    'df.Protons' column and find the column that matches with
    'proton'. If the row that contains 'proton' also contains
70     'Isotope' in the 'df.Isotope' column, then the value stored
    in 'df.Relative_Atomic_Mass' is reported for that row.
    Because the proton numbering scheme can have a format
    '10' for hydrogen and '10' for neon (following MCNP ZAID
    naming conventions) if we don't find a value with the whole
75     string of 'proton' then the program looks through the first

```

```

    element of string and tries to match that 'proton[0]'
    If no matches are found, and error is thrown out.

    df = dataset with columns 'Protons' 'Isotopes' and
80    'Relative_Atomic_Mass'. Dataset created with pandas

    proton = string with proton number (follow MCNP zaid format)

    Isotope = string with isotope number (just put the atomic mass
85    do not follow MCNP format - different for few cases)
    """
    #print(df)
    for i in range(0, len(df.Protons)):
        dfPro=str(df.Protons[i])
90        if proton==dfPro:
            dfIso=str(df.Isotope[i])
            if Isotope==dfIso:
                Mass=df.Relative_Atomic_Mass[i]
                break

95    try:
        Mass
    except NameError:
        for i in range(0, len(df.Protons)):
            dfPro=str(df.Protons[i])
100            if proton[0]==dfPro:
                dfIso=str(df.Isotope[i])
                if Isotope==dfIso:
                    Mass=df.Relative_Atomic_Mass[i]
                    break

105    try:
        Mass
    except NameError:
        print("Could not find atomic mass for proton = "\
            +proton+" and for Isotope = "+Isotope)
110    Mass=ReturnUfloat(Mass)
    return(Mass)

def CheckInParen(i, ChemicalFormula):
    """
115    i = index inside the string 'ChemicalFormula'
    ChemicalFormula = string that could potentially have ()

    Please note, this code is not complete
    """
    NumberOpenParen=ChemicalFormula.count("(")
    NumberCloseParen=ChemicalFormula.count(")")
    if NumberOpenParen != NumberCloseParen:
        print("Unbalanced parentheses in chemical formula")
        quit()
125    if NumberOpenParen==0:
        return(1, False)

    print("Hello")

```



```

Mul=4
130 Test=True
    return (Mul,Test)

def ChemList (ChemicalFormula):
    """
135     This function will take in a string for a
        chemical formula.

        Please modify your formula to fit the following rules

140     1. No repeats of elements (sum up all the same time element)
        2. To enter a subscript use "_", for example He_3 indicates
            three helium atoms.
        3. Use captical letters for the first letter of an element.
            If there are multiple letters for an elemental symbol,
145     then use lowercase for the second letter (program does
            not interpret three symbol elements)
        4. If there are more than 999 of a single atom in your chemical
            formula, you will have to write your own code. Or modify
            this one.
150     """
    i=0
    List=[]
    while (i <len(ChemicalFormula)-1):
        start=i
155         #print("The beginning i index = "+str(i))
        if re.search('[A-Z]',ChemicalFormula[i]):           #Capital letter?
            if re.search('[a-z]',ChemicalFormula[i+1]):     #Followed by lowercase?
                if re.search('_',ChemicalFormula[i+2]):     #Followed by more than 1?
                    if re.search('[0-9]',ChemicalFormula[i+5]): #Hundreds check
160                     List=np.append(List,ChemicalFormula[i:i+6])
                        #print (ChemicalFormula[i:i+6])
                        i=i+6
                    elif re.search('[0-9]',ChemicalFormula[i+4]): #tens check
                        List=np.append(List,ChemicalFormula[i:i+5])
165                         #print (ChemicalFormula[i:i+5])
                        i=i+5
                    else:                                     #If not hundres or tens, then c
                        List=np.append(List,ChemicalFormula[i:i+4])
                        #print (ChemicalFormula[i:i+4])
170                         i=i+4
                else:                                       #If not more than one, print
                    List=np.append(List,ChemicalFormula[i:i+2])
                    #print (ChemicalFormula[i:i+2])
                    i=i+2
            elif re.search('_',ChemicalFormula[i+1]):      #If only single symbol, then do
175                 if re.search('[0-9]',ChemicalFormula[i+4]): #hundreds
                    List=np.append(List,ChemicalFormula[i:i+5])
                    #print (ChemicalFormula[i:i+5])
                    i=i+5
            elif re.search('[0-9]',ChemicalFormula[i+3]):  #tens
180                 List=np.append(List,ChemicalFormula[i:i+4])

```

```

        #print (ChemicalFormula[i:i+4])
        i=i+4
    else:
        List=np.append(List,ChemicalFormula[i:i+3])
        #print (ChemicalFormula[i:i+3])
        i=i+3
    else:
        List=np.append(List,ChemicalFormula[i])
        #print (ChemicalFormula[i])
        i=i+1
    if start==i: #If we didn't find anything useful
        i=i+1
    #print("The end i index = "+str(i))
195 return (List)

def StringToMass(string):
    """
    This function takes in a string of the form
    200 zaid fraction error zaid fraction error ...
    will read a file called 'AtomicWeights.csv'
    and find the atomic weight with error of the zaid
    and store those value in a list called Mass
    """
    205 ListOfString=string.split()

    if not len(ListOfString)%3==0:
        print ("Check string variable missing fraction or error")
        quit()

    210 #Initialize fractions and zaid
    Zaid=0*np.arange(0,int(len(ListOfString)/3))

    #Gather fraction data and zaid data
    215 for i in range(0,int(len(ListOfString)/3)):
        Zaid[i]=int(ListOfString[i*3])

    df = pd.read_csv('../Data/AtomicWeights.csv')
    220 #Gather Mass Data
    for i in range(0,len(Zaid)):
        sZaid=str(Zaid[i])
        if len(sZaid)==4:
            proton=sZaid[0:2]
            225 if sZaid[2]=="0":
                Isotope=sZaid[3]
            else:
                Isotope=sZaid[2:4]
        elif len(sZaid)==5:
            230 proton=sZaid[0:2]
            if sZaid[2]=="0":
                Isotope=sZaid[3:5]
            if sZaid[3]=="0":
                Isotope=sZaid[4:5]

```

```
235         if sZaid[2]!="0" and sZaid[3]!="0":
            Isotope=sZaid[2:5]
        elif len(sZaid)==6:
            proton=sZaid[0:3]
            Isotope=sZaid[3:6]
240     else:
        print("Length of zaid is not 4 5 or 6 err")
        quit()
    try:
        Mass=np.append(Mass,FindAtomicMass(df,proton,Isotope))
245    except NameError:
        Mass=FindAtomicMass(df,proton,Isotope)

    return (Mass,Zaid)

250 def StringToMass2(string):
    """
    This function takes in a string of the form
    zaid fraction error zaid fraction error ...
    will read a file called 'AtomicWeights.csv'
255    and find the atomic weight with error of the zaid
    and store those value in a list called Mass
    """
    ListOfString=string.split()

260    if not len(ListOfString)%3==0:
        print("Check string variable missing fraction or error")
        quit()

    #Initialize fractions and zaid
265    Zaid=0*np.arange(0,int(len(ListOfString)/3))

    #Gather fraction data and zaid data
    for i in range(0,int(len(ListOfString)/3)):
        Zaid[i]=int(ListOfString[i*3])
270        floatednumber=ufloat(float(ListOfString[i*3+1]),
                                float(ListOfString[i*3+2]))

        try:
            AtomFractions=np.append(AtomFractions,floatednumber)
        except NameError:
275            AtomFractions=floatednumber

    df = pd.read_csv('../Data/AtomicWeights.csv')
    #Gather Mass Data
    for i in range(0,len(Zaid)):
280        sZaid=str(Zaid[i])
        if len(sZaid)==4:
            proton=sZaid[0:2]
            if sZaid[2]=="0":
                Isotope=sZaid[3]
285        else:
            Isotope=sZaid[2:4]
        elif len(sZaid)==5:
```

```

        proton=sZaid[0:2]
        if sZaid[2]=="0":
290             Isotope=sZaid[3:5]
        if sZaid[3]=="0":
            Isotope=sZaid[4:5]
        if sZaid[2]!="0" and sZaid[3]!="0":
            Isotope=sZaid[2:5]
295     elif len(sZaid)==6:
        proton=sZaid[0:3]
        Isotope=sZaid[3:6]
    else:
        print("Length of zaid is not 4 5 or 6 err")
300        quit()
    try:
        Mass=np.append(Mass,FindAtomicMass(df,proton,Isotope))
        protons=np.append(protons,proton)
    except NameError:
305        Mass=FindAtomicMass(df,proton,Isotope)
        protons=proton

    return (Mass,protons,AtomFractions)

310 def ConvertFractions(string,Mass,MasstoAtom,Zaid):
    """
    This function will convert, with error, the mass or atom fraction
    to the other (mass to atom or atom to mass). It will use the masses
    provided in Mass, and the fractions provided in string. If its mass to Atom then
315    MasstoAtom=True, otherwise set False
    """

    ListOfString=string.split()
    Total=ufloat(0.,0)

320     for i in range(0,len(Zaid)):

        Fraction=ufloat(float(ListOfString[i*3+1]),float(ListOfString[i*3+2]))
        if MasstoAtom: #Calculate total Atoms
325             Total=Total+Fraction/Mass[i]
        else: #Calculate total Mass
            Total=Total+Fraction*Mass[i]

    stringCalculated=''
330     for i in range(0,len(Zaid)):

        Fraction=ufloat(float(ListOfString[i*3+1]),float(ListOfString[i*3+2]))
        if MasstoAtom:
            #Calculate atom fractions
335             FractionCalculated=(Fraction/Mass[i])/Total
        else:
            #Calculate mass fractions
            FractionCalculated=(Fraction*Mass[i])/Total

340     stringCalculated=stringCalculated+

```

```

        str(Zaid[i])+' '+\
        str(FractionCalculated)+' '

    return (stringCalculated)
345

def FindSymbol (NumofProtons,df) :
    """
    This function will find the element symbol, based on number of
350 protons.
    """
    for i in range(0,len(df.Protons)):
        if str(df.Protons[i])==NumofProtons:
            Symbol=df.Symbol[i]
355         break

    try:
        Symbol
    except NameError:
360         print ("Could not find Symbol for Modification zaid")
        quit()

    return (Symbol)

365 def FormatMods (Modifications,df) :
    """
    This functions formats modifications

    """
370     for i in range(0,len(Modifications)):
        Modifications[i]=Modifications[i].replace('+/-',' ')

        Mass,protons,AtomFractions=StringToMass2 (Modifications[i])
        Mass=" ".join(str(i) for i in Mass)
375         protons=" ".join(str(i) for i in protons)
        LAtomFractions=" ".join(str(i) for i in AtomFractions)
        try:
            ModMass=np.append (ModMass,Mass)
            Modprotons=np.append (Modprotons,protons)
380             ModAFrac=np.append (ModAFrac,LAtomFractions)
        except NameError:
            ModMass=[Mass]
            Modprotons=[protons]
            ModAFrac=[LAtomFractions]
385

    for i in range(0,len(Modifications)):
        proton=Modprotons[i].split(" ")[0]
        symbol=FindSymbol (proton,df)
390     try:
        ModSymbols=np.append (ModSymbols,symbol)
    except NameError:
        ModSymbols=symbol

```

```

395     return (ModMass, ModSymbols, ModAFrac)

def DetermineMolarMass(List, df, ModSymbols,
                        ModMass, AtomFractions,
                        ChemicalFormulaError):
400     """
        this function determines the molar mass of a chemical formula
        with error:
        List is a list of the chemical formula
        df is a dataframe with atomic mass information
405     ModSymbols are the modificaition symbols (if using different Dudes
        AtomFractions are the atom fractions of the different dudes
        ChemicalFormulaError is the error in the number of each atom in the
        chemical formula, for example UO_2 could have a chemical formula
        ChemicalFormulaError=[0,0.001], meaning that a very small amount of
410     the time, we have UO_3...this isn't the best way of doing this...
        """
    MolarMass=ufloat(0,0)
    for i in range(0, len(List)):
        Symbol=List[i].split("_")[0]
415         try:
            Multiplier=List[i].split("_")[1]
        except IndexError:
            Multiplier=1
        Multiplier=ufloat(Multiplier, ChemicalFormulaError[i])
420         for j in range(0, len(df.Symbol)):
            if Symbol==str(df.Symbol[j]):
                ModifyElement=False
                for k in range(0, len(ModSymbols)):
                    if ModSymbols[k]==Symbol: #We are modifying
425                         ModifyElement=True
                        Masses=ModMass[k].split(" ")
                        AFractions=AtomFractions[k].split(" ")
                        IndividualMolarMass=0
                        for l in range(0, len(Masses)):
430                             IndividualMolarMass=IndividualMolarMass+\
                                ReturnUfloat(Masses[l])*\
                                ReturnUfloat(AFractions[l])

                if not ModifyElement:
                    IndividualMolarMass=ReturnUfloat(
435                         df.Standard_Atomic_Weight[j]
                    )

                # print(Symbol+" "+
                #         str(IndividualMolarMass)
                #         )
440             MolarMass=MolarMass+IndividualMolarMass*Multiplier
            break
    return (MolarMass)

def FindRange(List, Item):
445     """
        This function returns a range...yup
    """

```

```

    """
    for i in range(0, len(List)-1):
        if List[i] == Item:
450             Range=[List[i]]
                break
        elif List[i+1] == Item:
            Range=[List[i+1]]
                break
455         elif List[i] <= Item <= List[i+1]:
            Range=[List[i],List[i+1]]
                break
    return (Range)

460 def FindInTable(List1,List2,ItemMatchWithList2):
    """
    This function needs two lists that are the same
    length. and with data that corresponds to each other
    searches through list2 to find the item,
465     then reports that same value from list1
    """
    for i in range(0, len(List2)):
        if (ItemMatchWithList2==List2[i]):
            return (List1[i])

470 def InterpolateDensity(dfDen,Temp,TRange,Conc,CRange):
    """
    This function interpolates stuff...don't ask me how
    """
475     Concentrations=dfDen['Concentration_Percent_Weight']

    for i in range(0, len(TRange)):
        t=dfDen[str(int(TRange[i]))+' C']
        for j in range(0, len(CRange)):
480             C=CRange[j]
                D=FindInTable(t,Concentrations,C)
                try:
                    Densities=np.append(Densities,D)
                except NameError:
485                     Densities=[D]

    if len(Densities)==4:
        Q11=((TRange[1]-Temp)*(CRange[1]-Conc))/\
            ((TRange[1]-TRange[0])*(CRange[1]-CRange[0]))
490        Q21=((Temp-TRange[0])*(CRange[1]-Conc))/\
            ((TRange[1]-TRange[0])*(CRange[1]-CRange[0]))
        Q12=((TRange[1]-Temp)*(Conc-CRange[0]))/\
            ((TRange[1]-TRange[0])*(CRange[1]-CRange[0]))
        Q22=((Temp-TRange[0])*(Conc-CRange[0]))/\
495            ((TRange[1]-TRange[0])*(CRange[1]-CRange[0]))

        density=Q11*Densities[0]+Q12*Densities[1]+\
            Q21*Densities[2]+Q22*Densities[3]

```

```

500     if len(Densities)==1:
        density=Densities[0]

    if len(Densities)==2:
        if len(TRange)==2:
505             density=( (Temp-TRange[0]) * (Densities[1]-Densities[0])) /\
                (TRange[1]-TRange[0]) +Densities[0]
            if len(CRange)==2:
                density=( (Conc-CRange[0]) * (Densities[1]-Densities[0])) /\
                    (CRange[1]-CRange[0]) +Densities[0]
510
        #print(density)
        #print(Temp)
        #print(Conc)
        return(density)
515
def GetDensity(Temperature,WtConcentration,dfDen):
    """
    This function gets you density, don't ask me how
    """
520    MinTemp=Temperature.nominal_value-Temperature.std_dev
    MaxTemp=Temperature.nominal_value+Temperature.std_dev
    MinWtCon=WtConcentration.nominal_value-WtConcentration.std_dev
    MaxWtCon=WtConcentration.nominal_value+WtConcentration.std_dev

525    Columns=list(dfDen.columns.values)

    #Find all the temperatures
    for i in range(0,len(Columns)):
        if (' C ' in Columns[i]):
530            Temp=float(Columns[i].split(" C ")[0])
            try:
                TempsAva=np.append(TempsAva,Temp)
            except NameError:
                TempsAva=Temp
535

    #Find the temperatures you fit between
    MinTempRange=FindRange(TempsAva,MinTemp)
    MaxTempRange=FindRange(TempsAva,MaxTemp)

540    #Find all the concentrations
    for i in range(0,len(dfDen.Concentration_Percent_Weight)):
        StrCon=float(dfDen.Concentration_Percent_Weight[i])
        try:
            Concentration=np.append(Concentration,StrCon)
545        except NameError:
            Concentration=StrCon

    #Find concentrations you fit between
    MinConRange=FindRange(Concentration,MinWtCon)
550    MaxConRange=FindRange(Concentration,MaxWtCon)

    density=InterpolateDensity(dfDen,

```



```

555         MinTemp,
            MinTempRange,
            MinWtCon,
            MinConRange)

    density=np.append(density, InterpolateDensity(dfDen,
                                                    MinTemp,
560                                                    MinTempRange,
                                                    MaxWtCon,
                                                    MaxConRange) )

    density=np.append(density, InterpolateDensity(dfDen,
                                                    MaxTemp,
565                                                    MaxTempRange,
                                                    MinWtCon,
                                                    MinConRange) )

    density=np.append(density, InterpolateDensity(dfDen,
                                                    MaxTemp,
570                                                    MaxTempRange,
                                                    MaxWtCon,
                                                    MaxConRange) )

575    densityN=(max(density)+min(density))/2
    densityE=densityN-min(density)
    density=ufloat(densityN,densityE)
    return(density)

580 def ConvertMol(MolarityToMolality,First,
                gramsOmol,dfDen,Temperature):
    """
585    This function will convert molality to molarity
    and viceversa
    """
    #First either equals Molarity or Molality
    #Second either equals Molarity or Molality
    if not MolarityToMolality:
590        WtConcentration=100/(1000/(First*gramsOmol)+1)
    else:
        dif=1
        WtConcentration=ufloat(30,0.1) #A Guess
        while( abs(dif)>0.001):
595            OldWt=WtConcentration
            density=GetDensity(Temperature,OldWt,dfDen)
            WtConcentration=(100*gramsOmol*First)/(1000*density)
            dif=(WtConcentration-OldWt)/WtConcentration

600    density=GetDensity(Temperature,WtConcentration,dfDen)

    #####
    ##### Calculation #####
    #####
605

```

```

        if MolarityToMolality:
            # (mols/kg)
            #dif=1
            #while (abs(dif)>0.001):
610         #NewSecond=1/(density/First-gramsOmol*0.001)
            #WtConcentration=100/(1000/(NewSecond*gramsOmol)+1)
            #density=GetDensity(Temperature,WtConcentration,dfDen)
            #Second=1/(density/First-gramsOmol*0.001)
            #dif=Second-NewSecond
615         Second=1/(density/First-gramsOmol*0.001)
        else:
            # (mols/L)
            Second=density/(1/First+gramsOmol*0.001)

620     return (Second)

def NewConcentration(m1,m2,gramsOmol,
                    Temperature,dfDen,
                    Vol1,Vol2):
625     """
        This function calculates a new concentration when
        two volumes of the same substance are added together
        same temperature, assuming that both solutions
        have had time to cool
630     """

    WtConcentration1=100/(1000/(m1*gramsOmol)+1)
    WtConcentration2=100/(1000/(m2*gramsOmol)+1)

635    p1=GetDensity(Temperature,WtConcentration1,dfDen)
    p2=GetDensity(Temperature,WtConcentration2,dfDen)

    molsV1=(m1*gramsOmol*p1*Vol1)/(1000*gramsOmol+m1*(gramsOmol**2))
    molsV2=(m2*gramsOmol*p2*Vol2)/(1000*gramsOmol+m2*(gramsOmol**2))
640

    #kgSol1=(1000*p1*Vol1)/(1000+m1*gramsOmol)/1000
    #kgSol2=(1000*p2*Vol2)/(1000+m2*gramsOmol)/1000

    kgSol1=(1-WtConcentration1/100)*(p1*Vol1)/(1000)
645    kgSol2=(1-WtConcentration2/100)*(p2*Vol2)/(1000)

    Totmols=molsV1+molsV2
    Totkg=kgSol1+kgSol2

650    m3=Totmols/Totkg
    WtConcentration3=100/(1000/(m3*gramsOmol)+1)
    #Assuming its had time to cool down
    p3=GetDensity(Temperature,WtConcentration3,dfDen)
    Vol3=(p1*Vol1+p2*Vol2)/p3
655

    Molarity=ConvertMol(False,m3,gramsOmol,dfDen,Temperature)

    return (m3,p3,Vol3,WtConcentration3,Molarity)

```

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Problem 2

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Example Figure

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This is an example citation [1].

References

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