Applications of Computer Science in Environmental Models

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Abstract: **- Computation is now regarded as an equal and indispensable partner, along with theory and experiment, in the advance of scientific knowledge and engineering practice. Numerical simulation enables the study of complex systems and natural phenomena that would be too expensive or dangerous, or even impossible, to study by direct experimentation. The quest for ever higher levels of detail and realism in such simulations requires enormous computational capacity, and has provided the impetus for dramatic breakthroughs in computer algorithms and architectures. Due to these advances, computational scientists and engineers can now solve large-scale problems that were once thought intractable. Computational science and engineering (CSE) is a rapidly growing multidisciplinary area with connections to the sciences, engineering, and mathematics and computer science. CSE focuses on the development of problem-solving methodologies and robust tools for the solution of scientific and engineering problems. We believe that CSE will play an important if not dominating role for the future of the scientific discovery process and engineering design. The computation science is now being used widely for environmental engineering calculations. The behavior of environmental engineering systems and processes can be studied with the help of computation science and understanding as well as better solutions to environmental engineering problems can be obtained.**

Key Words: **algorithms, computation, environmental engineering, simulation.**

I. INTRODUCTION

Chemistry. Computational chemistry (CC) is widely used in academic and industrial research. Computed molecular structures, e.g., very often are more reliable than experimentally determined ones. According to "Chemical & Engineering News," the newsletter of the American Chemical Society, Computational Chemistry has developed from a "nice to have"' to a "must-have"' tool . The main incentive of CC is the prediction of chemical phenomena based on models which relate either to first principles theory ("rigorous models"), to statistical ensembles governed by the laws of classical physics or thermodynamics, or simply to empirical knowledge. In real problem solving situations, these models are often combined to form "hybrid models" where only the critical part of the problem is treated at the rigorous level of theory. Rigorous theory in the molecular context is synonymous with quantum mechanics, i.e., solving the Schrödinger equation for a molecular complex with or without the presence of external perturbation (photons, electric fields, etc.). There are a number of methods available which provide approximate solutions to the Schrödinger equation (Hartree - Fock and Density Functional theory, e.g.). Simulation is used to predict properties of large and complex entities such as a liquid, the folding of a protein in solution, or the elasticity of a polymer. Finally, empirical models most often try to establish correlations between the structure of a molecule and its (pharmaceutical) activity. Simulations and quantum chemical calculations, on the other hand, very often are extremely compute-intensive due to the number of degrees of freedom and the complexity of the terms to be evaluated. The high accuracy required in these calculations sets restrictions with regard to the method used to solve the partial differential equations (PDEs) involved. Further information is available at the website for the International Union of Pure and Applied Chemistry.

Bio engineering. Historically, engineers have used chemistry, thermodynamics, and transport to design chemical processes. Now these fundamental processes are applied to the understanding of complex biological phenomena that are governed by the same physical laws. Computer models are being used to understand and to develop treatments for glaucoma, to understand and to fabricate bio artificial materials for example bio artificial arteries, and for studying the normal and pathologic response of soft hydrated tissues in the human musculoskeletal system.

II. APPLICATION OF COMPUTATIONAL SCIENCE IN ENVIRONMENTAL ENGINEERING

Computational science as mentioned above can be used in multiple areas for the inter conversion of data to obtain a final software program. This has been shown in detail with a case study below.

A. Materials and Methods

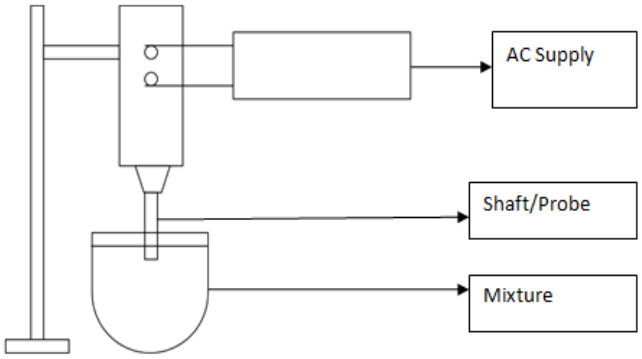


Fig 1 Batch sonication process

Sonication is a process of advanced oxidation in which the sample solution is irradiated with the ultrasonic waves (A.S. Stasinakis2005, Mira Petrovic, 2011) . The reactor used in this case is the probe reactor. The irradiation causes physical, chemical and biological changes in the water.(K. S. Gandhi and R. Kumar 1994, Kenneth S. Suslick, 1999, L. H. Thompson and L.K.Doraiswamy 1999, Uma Mukherji, 2003). It is seen that the process also affects the Chemical Oxygen Demand which was verified using standard method (APHA, 2005).

The solution of aspirin having concentration of 700 mg/L was prepared by adding two disprin tablets to 1000 ml deionised water of laboratory grade. The single tablet of aspirin contains 350 mg aspirin by weight. The tablet is self dispersible and dissolves by itself. A slight stirring may be done at the end with a glass rod if required. The detailed pre-sonication observations for this concentration have been reported in table 1 below.(Royal Society of Chemistry, 2003, R.K. Maheswari et al. 2010)

B Observations

Table 1 Presonication sample parameters observed

S. No	Parameter Observed	Observed Value
1.	pH	3.1
2.	Total Dissolved Solids TDS	152 ppm
3.	Conductivity	200 µS/cm
4.	Sample Volume	500 ml
5.	Sonication Frequency	20 kHz
6.	Sonication Mode	Continuous
7.	Initial Concentration of Sample	700 mg/L

Table 2 postsonication sample parameters observed

S. No	Amplitude of Sonication in %	Time of sonication In mints in minutes	End point of titration for non sonicated sample in ml	End point of titration for sonicated sample in ml	% Aspirin at start of sonication 700 mg/L	% Aspirin Degraded at the end of sonication
1.	10	05	2.3	1.2	100	47.83
2.	20	05	2.3	0.8	100	65.22
3.	30	05	2.3	0.7	100	69.57
4.	40	05	2.3	0.7	100	69.57
5.	50	05	2.3	0.6	100	73.92
6.	60	05	2.3	0.5	100	78.27
7.	70	05	2.3	0.4	100	82.61
8.	80	05	2.3	0.4	100	82.61
9.	90	05	2.3	0.4	100	82.61
10	100	05	2.3	0.3	100	86.96
11.	10	10	2.3	0.5	100	78.27
12.	20	10	2.3	0.5	100	78.27
13.	30	10	2.3	0.5	100	78.27
14.	40	10	2.3	0.4	100	82.61
15.	50	10	2.3	0.4	100	82.61
16.	60	10	2.3	0.4	100	82.61
17.	70	10	2.3	0.3	100	86.96
18.	80	10	2.3	0.3	100	86.96
19.	90	10	2.3	0.2	100	91.30
20	100	10	2.3	0.2	100	91.30
21.	10	15	2.3	0.4	100	82.61
22.	20	15	2.3	0.2	100	91.30
23.	30	15	2.3	0.2	100	91.30
24.	40	15	2.3	0.2	100	91.30
25.	50	15	2.3	0.2	100	91.30
26.	60	15	2.3	0.2	100	91.30
27.	70	15	2.3	0.2	100	91.30
28.	80	15	2.3	0.2	100	91.30
29.	90	15	2.3	0.2	100	91.30
30.	100	15	2.3	0.2	100	91.30

C Program development in C++

If a value for biodegradation was reported as the % BOD (Biochemical Oxygen Demand) or as the percentage of chemical degraded then this information can be converted to a half-life estimate. Assuming first order decay from an initial quantity C_0 to C_a in time t gives (Jon Arnot et al., 2005, P. C. Jain 2013, Charles G hill Jr., Thatcher Root, 2003, Salil K. Ghoshal 1997)

$$C_a = C_0 \exp. (-kt) \quad (1)$$

Where, k is the reaction rate constant. The percent loss or BOD is then

$$BOD = 100 \times (C_0-C_a/C_0) = 100 \times (1- \exp.) (- kt) \quad (2)$$

From which k can be calculated as

$$k = (-1/t) \ln (100 - \% BOD/100) \quad (3)$$

The half life $t_{1/2}$ is then 0.693/k or

$$t_{1/2} = - 0.693\ t/\ln (100 - \% BOD / 100) \quad (4)$$

This is the case for kinetic modeling (Catherine A. Peters 2001, Yanhui Hu, 2011)

D Sample data

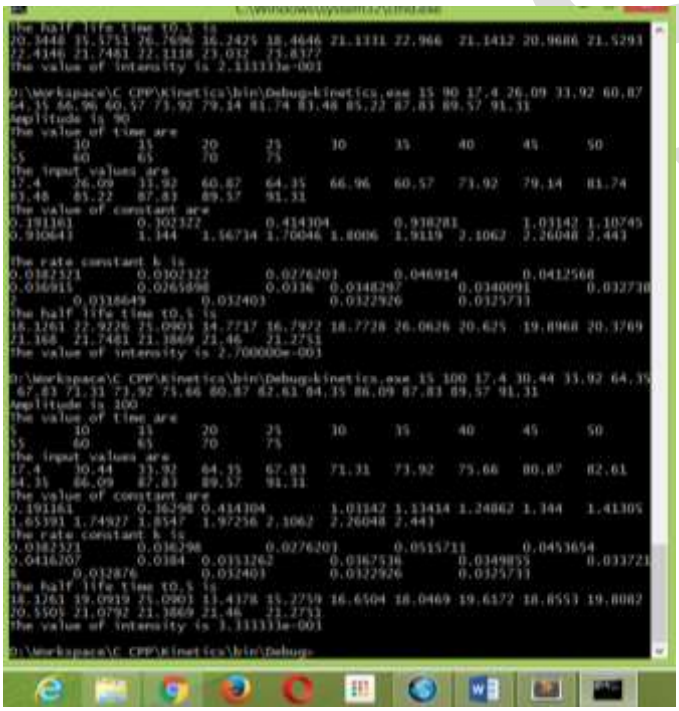
C++ Program

```
#include<iostream>
#include<math.h>
#include<stdlib.h>
#include <fstream>
#include<string>
#include <iomanip>
using namespace std;
int main(int argc, char *argv[])
{
if(argc!=(atoi(argv[1])+3))
   {
cout<<"Enter appropriate arguments";
exit(1);
   }
else
   {
int i,a;
      double k[15],t[15],x[15],h[15],p,c[15];
      a= atoi(argv[2]);
cout<<"Amplitude is "<<a<<endl;
cout<<"The value of time are\n";
for(i=0;i<atoi(argv[1]);i++)
      {
t[i]=5+i*5;
cout<<t[i]<<"\t";
      }
cout<<endl;
cout<<"The input values are"<<endl;
for(i=0;i<atoi(argv[1]);i++)
      {
x[i]= atof(argv[i+3]);
cout<<x[i]<<"\t";
      }
cout<<endl;
for(i=0;i<atoi(argv[1]);i++)
      {
c[i]=log(100/(100-x[i]));
k[i]=(1/t[i])*c[i];
h[i]=0.693/k[i];
      }
cout<<"The value of constant are\n";
for(i=0;i<atoi(argv[1]);i++)
      {
cout<<c[i]<<"\t";
      }
cout<<endl;
cout<<"The rate constant k is\n";
for(i=0;i<atoi(argv[1]);i++)
      {
cout<<k[i]<<"\t";
      }
cout<<endl;
cout<<"The half life time t0.5 is\n";
for(i=0;i<atoi(argv[1]);i++)
      {
cout<<h[i]<<"\t";
      }
cout<<endl;
      p=(a*a)/double(2*1000*1500);
cout<<"The value of intensity is "<<scientific<<p<<endl;
ofstream outdata;
outdata.open("readings.csv", ios::app);
outdata<<"Table for amplitude "<<a<<endl<<endl;
outdata<<"Time of Sonication"<<",";
for(i=0;i<atoi(argv[1]);i++)
      {
outdata<< t[i];
outdata<< ",";
      }
outdata<<endl;
outdata<<"% Aspirin at end of Sonication"<<",";
for(i=0;i<atoi(argv[1]);i++)
      {
outdata<< x[i];
outdata<< ",";
      }
outdata<<endl;
outdata<<"Value of ln(C0/Ca"<<",";
for(i=0;i<atoi(argv[1]);i++)
      {
outdata<< c[i];
```

```
outdata<< ",";
      }
outdata<<endl;
outdata<<"Value of constant k"<<",";
for(i=0;i<atoi(argv[1]);i++)
      {
outdata<< k[i];
outdata<< ",";
      }
outdata<<endl;
outdata<<"Value of half life t0.5"<<",";
for(i=0;i<atoi(argv[1]);i++)
      {
outdata<< h[i];
outdata<< ",";
      }
outdata<<endl<<endl;
outdata<<"Values                                    of
intensity"<<scientific<<p<<endl<<endl<<endl<<endl;
outdata.close();
return 0;
   }

}
```

Data obtained in terms of rate constant (k) and half life (t1/2) using above program in C++



Data obtained for rate constant (k) and half life (t1/2) for different amplitudes of sonication.

III. CONCLUSIONS

The program in C++ was successfully developed and utilized for calculations relating to both Chemical Engineering and Civil Engineering (Environmental Engineering). It did not only simplify the work but this progam can now be used to make any number of calculations. The data thus obtained can be modeled and validated.

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