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ARSEPPA: A Visual Basic software tool for arsenic separation plant performance analysis

P. Pal[a,*], Z. Ahammad[a], P. Bhattacharya[b]

[a] *Department of Chemical Engineering, National Institute of Technology, Durgapur 713209, India*
[b] *Department of Chemical Engineering, Jadavpur University, Calcutta 700032, India*

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Abstract

A Visual Basic software ('ARSEPPA') in Microsoft Excel environment has been developed for the first time for performance analysis of arsenic separation plants in the backdrop of absence of such a software. The user-friendly, menu-driven add-in in Excel is based on dynamic mathematical model developed for the systematically integrated physico-chemical processes involved in removal of arsenic from drinking water. The software has been validated by carrying out extensive investigation in a laboratory-scale experimental set up and by comparing the experimental findings with the software-predicted values. An overall correlation coefficient of the order of 0.98890 has been obtained indicating the capability of the software in analyzing plant performance with reasonable accuracy. The software does not require familiarity with any new environment and through visual graphics, it permits very quick performance analysis of the individual units as well as the overall process. Flexibility in input data manipulation and capability of optimization of the major operating variables are the other advantages of the software. The simulation package is expected to be extremely useful in raising the level of confidence in designing and operating arsenic separation plants.

Keywords: Arsenic separation; Physico-chemical processes; Visual Basic software; Excel environment

1. Introduction

Contamination of ground water by arsenic that mainly leaches out from its crystal lattice due to geological disturbances is now a world-wide environmental problem being faced by millions of people in Chile [1], South-West U.S.A., Taiwan, Bangladesh, Nepal and India. Such contamination of ground water by arsenic in several parts of the world and epidemiological evidence of arsenic carcinogenicity have necessitated stringent regulation of arsenic concentration in potable water for protection of public health. WHO has set a standard of 10 ppb as maximum contaminant level (MCL) of arsenic in potable water. It is now a challenge to achieve this standard, particularly in the areas where ground water is the only source of drinking water and arsenic pollution is wide spread.

In adsorption based studies [2–5] several adsorbents have been examined for assessing effectiveness of arsenic separation from drinking water in small scale. For large scale treatment of arsenic-contaminated ground water in the arsenic-affected areas of the developing countries, there is hardly any alternative to physico-chemical coagulation–precipitation of arsenic from drinking water. Particularly, where the river is far away from such affected villages, this low cost technology is likely to be the most promising one. Physico-chemical separation through chemical coagulation and precipitation has been demonstrated by many researchers [6–12] as one of the most effective methods of arsenic separation.

From these studies it transpires that the most appropriate arsenic removal scheme should include in sequence one oxidation unit or reactor (with only $KMnO_4$ as oxidant), a coagulator or slow-mixing unit (with $FeCl_3$ as coagulant and provision for controlling pH), a flocculator or quick-mixing unit and a sedimentation unit followed by one sand filtration unit. Despite extensive research work on several techniques of arsenic separation over the decades, millions of people in the developing countries particularly in South East Asia still continue to drink water highly contaminated with arsenic. There is still very limited confidence in design and operation of a physico-chemical treatment plant for arsenic removal from water as is evident from operation of a very limited number of such plants. There is still

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[*] Corresponding author. Tel.: +91 9434469750.
E-mail address: parimalpal2000@yahoo.com (P. Pal).

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Nomenclature

A	is the reactor cross-sectional area
A_F	is the area of the filter bed
A_d	is the sedimentation unit area (m^2)
A_{QM}	is the area of the coagulator/flocculator (m^2)
C	is the floc concentration of the solution ($kmol/m^3$)
C_c	is the coagulant concentration ($kmol/m^3$) in the coagulator
C_r	is the oxidant concentration ($kmol/m^3$)
C_{r_i} and C_r	are the initial and instantaneous concentration of the oxidant ($kmol/m^3$)
C_u	is the sludge concentration ($kmol/m^3$)
C_{A_i} and C_A	are the concentration ($kmol/m^3$) of arsenic(III) at the inlet and arsenic(V) at the outlet of the reactor
$C_{QM_{A_i}}$, C_{QM_A}	are the concentrations ($kmol/m^3$) of arsenic at the inlet and outlet
$C_{QM_{floc}}$	is the concentration of the floc ($kmol/m^3$)
dz/dt	is the sedimentation rate (m/s)
D_r	is the reactor diameter (m)
D_P or D_{SM_f}	diameter of the floc (m) in the flocculator
D_{QM}	is the coagulator diameter (m)
D_{QM_f}	diameter of floc particles in the coagulator–flocculator
D_{QM_f}	is the average diameter of the floc particles in the coagulator–flocculator (m)
F_i, F_0	volumetric flow rates (m^3/s) of the feed and treated water, respectively
F_r	is the volumetric feed rate (stoichiometric) of oxidant
F_{QM_i}, F_{QM_o}, F_{C_i}	are the flow rates (m^3/s) of the feed water, treated water and coagulant
F_{si}	is the volumetric feed rate of aqueous solution in the sedimentation unit
g	gravitational constant (m/s^2)
G_1	is the average root mean square velocity gradient in the coagulator–flocculator (s^{-1})
h	is the liquid level in the reactor (m)
h_{QM}	is the liquid level in the coagulator (m)
k	is the second order reaction (oxidation) rate constant ($mol^{-1}\ s^{-1}$)
K_{QM}	is the assumed overall second order rate constant ($mol^{-1}\ s^{-1}$) of arsenic flocculation, adsorption, enmeshment and settling
L	is the cake thickness (m)
n_1, n_2	are the kinetic constants
m_1, m_2	are the reaction kinetic constants
M_{floc}	is the average molecular weight of floc (kg/kmol)
M_{A_s}, M_r, M_c, M_{floc}	are molecular weights of arsenic, oxidant, coagulant and average molecular weight of the floc (kg/kmol)
N_{Re}	Reynolds number
P	is the power (Nm/s)
$-\Delta P$	is the pressure drop through the filter medium and filter cake (N/m^2)
ΔP_f, ΔP_c and ΔP	are the pressure drop across filter medium, filter cake and total pressure drop across the bed
Q_0	is the over flow rate
R_m	is the filter medium resistance
S_p	specific density
V	is the volume of the reactor (m^3)
V_{actual}	is actual upward velocity of over flow water
V_F	is the volume of filtrate (m^3)
V_{QM}	is the volume of the coagulator (m^3)
U	is the average settling velocity of the floc particles (m/s)
U_1, U_2	are the particle settling velocities
W	is the solid concentration of the water to be filtered

Greek letters

α	is the specific cake resistance (m/kg)
ε	is the porosity of the filter bed
μ	is the viscosity of the aqueous system involved (Pa s)
μ	is the viscosity of the aqueous solution at the inlet of filter unit
μ_L	is the viscosity (cp) of the aqueous solution in the sedimentation unit
ν_L	kinematic viscosity (m^2/s)
ρ_i, ρ_o	are the densities (kg/m^3) of water
ρ_r	is the density of oxidant
ρ_s, ρ_L	are the densities of the particles and the aqueous solution
ρ_{C_i}	is the density of the coagulant (kg/m^3)
ρ_{QM_i}, ρ_{QM_o}	are the densities (kg/m^3) of the inlet and outlet aqueous solutions in the coagulator–flocculator

doubt as to the effectiveness and economy of such a treatment plant. Though research abounds physico-chemical separation of arsenic from drinking water, neither any systematic modeling and simulation work considering the most appropriate treatment scheme as outlined above nor any software development work on the concerned, integrated processes has yet been taken up in this vital area of drinking water purification. But this could be of great help in full-scale design and operation of arsenic separation plants. In this work, a Visual Basic simulation software has been developed based on dynamic mathematical modeling of all the systematically integrated physico-chemical processes of arsenic separation from drinking water. The software which is a result of integration of knowledge from Computer software Engineering and Environmental Engineering with Chemical Engineering permits a very quick performance analysis of the process units involved in the separation of arsenic from water. The major advantage of the user-friendly and menu-driven software is that it deals with a continuous process where one can observe the effects of all the major operating parameters on the effectiveness of arsenic separation. This in turn helps set the operating parameters at their optimum levels. This is a menu-driven add-in in Microsoft Excel environment. It, therefore, does not require familiarity with any new environment. The software permits pre-analysis manipulation of input data and, visualization of the out put in a familiar environment. Though developed for arsenic separation from drinking water, the software can be extended to separation of many other heavy metals like calcium, magnesium, iron, lead, etc. from water.

2. Development of the software

The software 'ARSEPPA' was developed following the steps as outlined below:

(i) In the first step, the mathematical model for the integrated physical and chemical processes was developed based on the theoretical understanding of the mechanisms involved.
(ii) In the second step, the physico-chemical model parameters were determined either experimentally or by using standard mathematical relations available in the literature.
(iii) Subsequently, appropriate numerical solution technique was chosen and the algorithm developed for the solution of the model equations.
(iv) In the final step, the software was validated through experimental investigation and comparison between the model-predicted values and the experimental findings.

2.1. Development of the mathematical model

Mathematical model was developed based on mass balance for each unit and the assumptions as given below:

(i) Arsenic co-precipitates from the aqueous solution as As(V)–$Fe(OH)_3$ following pre-oxidation of all trivalent arsenic into pentavalent form and subsequent adsorption onto ferric hydroxides as arsenic settles better in pentavalent form than in trivalent form [13].
(ii) Arsenic may be present in water both in trivalent as well as pentavalent forms.
(iii) Oxidation of trivalent arsenic into pentavalent form in presence of potassium permanganate follows a pseudo first order reaction [14].
(iv) Because of the quick mixing and dispersion requirements in the oxidation unit, the oxidation reactor may be assumed to be CSTR type reactor.
(v) Because of spatial as well as temporal variation of the fluid velocity in the system, flocculation of arsenic precipitates may be assumed to follow orthokinetic mechanism.
(vi) For orthokinetic flocculation mechanism, change of concentration of settling particles may be assumed to follow O'Melia [15].
(vii) The overall process of enmeshment of arsenic onto ferric hydroxides and subsequent settling may be assumed to follow a first order reaction kinetics in the backdrop of kinetic limitations and the difficulties in decoupling the interrelated phenomena.

2.1.1. Material balance for the oxidizer unit

Overall mass balance of aqueous solution in the reactor unit is given below.

Change in mass = mass of raw water$|_{\text{input}}$ − mass of treated water$|_{\text{output}}$:

$$\rho_o A\left(\frac{dh}{dt}\right) = F_i\rho_i + F_{r_i}\rho_{r_i} - F_o\rho_o \tag{1}$$

where ρ_i, ρ_o are the densities (kg/m^3) of water at the inlet and outlet, ρ_r is the density of oxidant, F_i, F_0 the volumetric flow rates (m^3/s) of the feed and treated water, respectively, F_r the volumetric feed rate (stoichiometric) of oxidant, A the reactor cross-sectional area and h is the liquid level in the reactor.

2.1.2. Component mass balance of arsenic

Change in arsenic(V) concentration = arsenic(III) concentration$|_{\text{input}}$ − arsenic(V) concentration$|_{\text{output}}$ + generation of arsenic(V):

$$\frac{d}{dt}(C_A V) = F_i C_{A_i} - F_o C_A + VkC_A^{n_1} C_r^{n_2} \tag{2}$$

where C_{A_i} and C_A are the concentration (kmol/m^3) of arsenic(III) at the inlet and arsenic(V) at the outlet of the reactor, C_r the oxidant concentration (kmol/m^3), k the second order reaction (oxidation) rate constant (mol^{-1} s^{-1}), n_1 the kinetic constant, and V is the volume of the reactor (m^3).

2.1.3. Component mass balance of oxidant

Change in oxidant concentration = oxidant concentration$|_{\text{input}}$ − accumulation of oxidant:

$$\frac{d}{dt}(C_r V_r) = F_{r_i} C_{r_i} - VkC_A^{n_1} C_r^{n_2} \tag{3}$$

where C_{r_i} and C_r are the initial and instantaneous concentration (kmol/m^3) of the oxidant and n_2 is the kinetic constant.

2.1.4. Coagulator and flocculator

Over all mass balance of the aqueous solution in the coagulator and flocculator units are given below.

Change in mass in the coagulator–flocculator = mass of the input stream + mass of the coagulant stream − mass of the output stream:

$$\rho_{QM_o} A_{QM}\left(\frac{dh_{QM}}{dt}\right) = F_{QM_i}\rho_{QM} + F_c\rho_{c_i} - F_{QM_o}\rho_{QM_o} \tag{4}$$

where ρ_{QM_i}, ρ_{QM_o} are the densities (kg/m^3) of the inlet and outlet aqueous solutions in the coagulator–flocculator, ρ_{C_i} the density of the coagulant (kg/m^3), A_{QM} the area of the coagulator/flocculator (m^2), F_{QM_i}, F_{QM_o}, F_{C_i} are the flow rates (m^3/s) of the feed water, treated water and coagulant.

2.1.5. Component mass balance of arsenic(V)

Change in concentration of arsenic(V) = arsenic(V) concentration$|_{\text{input}}$ − arsenic concentration$|_{\text{output}}$ − accumulation of arsenic(V):

$$\frac{\mathrm{d}}{\mathrm{d}t}(C_{\mathrm{QM_A}}V_{\mathrm{QM}}) = F_{\mathrm{QM_i}}C_{\mathrm{QM_{A_i}}} - F_{\mathrm{QM_o}}C_{\mathrm{QM_A}} - V_{\mathrm{QM}}k_{\mathrm{QM}}C_{\mathrm{QM_A}}^{m_1}C_{\mathrm{C}}^{m_2} \tag{5}$$

where $C_{\mathrm{QM_{A_i}}}$, $C_{\mathrm{QM_A}}$ are the concentrations (kmol/m^3) of arsenic at the inlet and outlet, C_{c} the coagulant concentration (kmol/m^3) in the coagulator, V_{QM} the volume of the coagulator (m^3), k_{QM} the assumed overall second order rate constant (mol^{-1} s^{-1}) of arsenic flocculation, adsorption, enmeshment and settling, and m_1, m_2 are the reaction kinetic constants.

2.1.6. Component mass balance of floc

Change in floc concentration = generation of floc in the outlet stream:

$$\frac{\mathrm{d}}{\mathrm{d}t}(C_{\mathrm{QM_{floc}}}V_{\mathrm{QM}}) = V_{\mathrm{QM}}K_{\mathrm{QM}}C_{\mathrm{QM_A}}^{m_1}C_{\mathrm{C}}^{m_2} - F_{\mathrm{QM_o}}C_{\mathrm{QM_{floc}}} \tag{6}$$

where $C_{\mathrm{QM_{floc}}}$ is the concentration of the floc (kmol/m^3).

2.1.7. Component mass balance of coagulant

Change in coagulant concentration = input concentration of coagulant − accumulation of coagulant:

$$\frac{\mathrm{d}}{\mathrm{d}t}(C_{\mathrm{c}}V_{\mathrm{QM}}) = F_{c_i}C_{c_i} - V_{\mathrm{QM}}k_{\mathrm{QM}}C_{\mathrm{QM_A}}^{m_1}C_{\mathrm{c}}^{m_2} \tag{7}$$

2.1.8. Total rate of fall of floc concentration

$$\frac{\mathrm{d}C_{\mathrm{QM_{floc}}}}{\mathrm{d}t} = -\frac{2}{3}E_1G_1D_{\mathrm{QM_f}}^3C_{\mathrm{QM_{floc}}}^2 \tag{8}$$

$$E_1 = \frac{E'}{6.023\times10^{23}} \quad \text{and} \quad E' = 6.023\times10^{23}$$

where $E_1 = 1$ mol^{-1}, G_1 (s^{-1}) is the average root mean square velocity gradient in the coagulator–flocculator. $D_{\mathrm{QM_f}}$ (m) is the average diameter of the floc particles in the coagulator–flocculator.

2.1.9. Sedimentation unit

$$\frac{\mathrm{d}z}{\mathrm{d}t} = \frac{G}{C_{\mathrm{u}}} - U \tag{9}$$

where

$$G = F_{\mathrm{si}}\frac{C}{A_{\mathrm{d}}}, \qquad C_{\mathrm{u}} = C_{\mathrm{QM_{floc}}}$$

F_{si} is the volumetric feed rate (m^3/s) of aqueous solution in the sedimentation unit, C the floc concentration of the solution (kmol/m^3), A_{d} the sedimentation unit area (m^2), C_{u} the sludge concentration (kmol/m^3), U the average settling velocity of the floc particles (m/s), dz/dt the sedimentation rate (m/s) and G having unit kmol/m^2 s.

2.1.10. Filtration unit

Filtrate flow rate:

$$\frac{\mathrm{d}V_{\mathrm{F}}}{\mathrm{d}t} = \left[\frac{\mu\alpha WV_{\mathrm{F}}}{A_{\mathrm{F}}^2(-\Delta P)} + \frac{\mu R_{\mathrm{m}}}{A_{\mathrm{F}}(-\Delta P)}\right]^{-1} \tag{10}$$

where V_{F} is the volume of filtrate (m^3), A_{F} the area of the filter bed, α the specific cake resistance (m/kg), W the solid concentration of the water to be filtered, μ the viscosity of the aqueous system involved (Pa s), R_{m} the filter medium resistance, and $(-\Delta P)$ is the pressure drop through the filter medium and filter cake (N/m^2).

2.1.11. Initial conditions

$$h = 0; \quad C_{\mathrm{A}} = C_{\mathrm{A_i}}; \quad C_{\mathrm{r}} = C_{\mathrm{r_i}}; \quad h_{\mathrm{QM}} = 0;$$
$$C_{\mathrm{QM}} = C_{\mathrm{QM_i}}; \quad C_{\mathrm{QM_{floc}}} = 0; \quad C_{\mathrm{C}} = C_{\mathrm{C_i}}; \quad h_{\mathrm{SM}} = 0;$$
$$C_{\mathrm{SM_{floc}}} = 0; \quad z = 0; \quad V_{\mathrm{F}} = 0$$

2.2. Determination of the physico-chemical parameters

2.2.1. Computation of flow rate and concentration of oxidant

The flow rate of the oxidant was determined using a factor considering the stoichiometry of the reaction.

For flow and stoichiometric feed rate of oxidant dose—$F_{\mathrm{r_i}} = f_1F_{\mathrm{i}}$, where $f_1 < 1$:

$$C_{\mathrm{r_i}} = \frac{F_{\mathrm{i}}E_{\mathrm{A_s}}C_{\mathrm{A_i}}M_{\mathrm{r}}}{M_{\mathrm{A_s}}F_{\mathrm{r_i}}E_{\mathrm{r}}} \tag{11}$$

where $E_{\mathrm{A_s}} : E_{\mathrm{r}} = 1 : 15$; $M_{\mathrm{A_s}}$, M_{r} are molecular weights of arsenic and oxidant, respectively.

The density of the treated water at the outlet was determined considering the average density of the feed raw water and the oxidant. It may be safely assumed that the density of the aqueous stream at the outlet is almost same as the density of the feed stream as the oxidant quantity is negligible with respect to the feed solution flow rate:

$$\rho_{\mathrm{o}} = \frac{F_{\mathrm{i}}\rho_{\mathrm{i}} + F_{r_{\mathrm{i}}}\rho_{r_{\mathrm{i}}}}{F_{\mathrm{i}} + F_{r_{\mathrm{i}}}}, \qquad F_0 = F_{\mathrm{i}} + F_{r_{\mathrm{i}}} \tag{12}$$

Cross-sectional area and volume of the reactor are computed as

$$A = \frac{\pi D_{\mathrm{r}}^2}{4}, \qquad V = hA \tag{13}$$

D_{r} is the reactor diameter (m), V the volume of the reactor (m^3), h is the height of the reactor (m).

2.2.2. Computation of root mean square velocity gradient (G) in the coagulator and flocculator

The root mean square velocity gradient (s^{-1}) in the coagulator and flocculator was computed using the empirical relation:

$$G = \sqrt{\frac{P}{\mu V}} \tag{14}$$

where P is the power in Nm/s, μ the viscosity of aqueous system involved in Pa s, V the volume of reactor in m^3 and G has the unit of s^{-1}.

2.2.3. Computation of average floc size (D_{QM_f}) in the coagulator–flocculator unit

Diameter of floc particles in the coagulator–flocculator was computed using the empirical relation:

$$D_{\mathrm{QM_f}} = \left(\frac{3}{2E_1G_1C_{\mathrm{QM_{floc}}}t}\right)^{1/3} \tag{15}$$

where G_1 is the root mean square velocity gradient in the coagulator (s^{-1}) and $D_{\mathrm{QM_f}}$ (m) is the floc diameter.

2.2.4. Computation of flow rate and concentration of coagulant

The flow rate of the coagulant was determined using a factor considering the stoichiometry of the reaction.

For low and stoichiometric feed rate of the coagulant dose—$F_{\mathrm{c_i}} = f_2F_{\mathrm{QM_i}}$, where $f_2 < 1$:

$$C_{\mathrm{c_i}} = \frac{F_{\mathrm{QM_i}}E_{\mathrm{A_s}}C_{\mathrm{A_o}}M_{\mathrm{c}}}{M_{\mathrm{A_s}}F_{\mathrm{c_i}}E_{\mathrm{c}}} \tag{16}$$

where $E_{\mathrm{A_s}} : E_{\mathrm{c}} = 1 : 50$; $M_{\mathrm{A_s}}, M_{\mathrm{c}}, M_{\mathrm{floc}}$ are molecular weights of arsenic, coagulant and average molecular weight of the floc, respectively.

Assuming negligible change in density of the aqueous stream as it passes from the inlet of the oxidizer unit to the outlet of the filter unit:

$$\rho_{\mathrm{QM_o}} = \frac{F_{\mathrm{QM_i}}\rho_{\mathrm{QM_i}} + F_{\mathrm{c_i}}\rho_{\mathrm{c_i}}}{F_{\mathrm{QM_i}} + F_{\mathrm{c_i}}} \tag{17}$$

$$F_{\mathrm{QM_o}} = F_{\mathrm{QM_i}} + F_{\mathrm{c_i}}, \qquad F_{\mathrm{QM_i}} = F_0, \qquad \rho_{\mathrm{QM_i}} = \rho_{\mathrm{o}} \tag{18}$$

Area and volume of the coagulator:

$$A_{\mathrm{QM}} = \frac{\pi D_{\mathrm{QM}}^2}{4} \quad \text{and} \quad V_{\mathrm{QM}} = h_{\mathrm{QM}}A_{\mathrm{QM}} \tag{19}$$

D_{QM} is the coagulator diameter (m), V_{QM} the volume of the coagulator (m^3), and h_{QM} is height of the coagulator (m).

2.2.5. Determination of settling velocity and superficial velocity in sedimentation unit

When $D_{\mathrm{P}} < 1$ mm and $N_{Re} < 1$, where $D_{\mathrm{P}} = D_{\mathrm{SM_f}}$:

$$U_1 = \frac{(\rho_{\mathrm{S}} - \rho_{\mathrm{L}})gD_{\mathrm{P}}}{18\mu_{\mathrm{L}}} \tag{20}$$

$$N_{Re} = \frac{D_{\mathrm{P}}^3\rho_{\mathrm{L}}(\rho_{\mathrm{S}} - \rho_{\mathrm{L}})g}{18\mu_{\mathrm{L}}^2} \tag{21}$$

When $D_{\mathrm{P}} > 1$ mm and $N_{Re} > 1$:

$$U_2 = \frac{(S_{\mathrm{P}} - 1)^{0.8}g0.8D_{\mathrm{P}}^{1.4}}{10\nu_{\mathrm{L}}^{0.6}} \tag{22}$$

$$N_{Re} = \frac{D_{\mathrm{P}}\rho\mathrm{L}U_2}{\mu_{\mathrm{L}}} \tag{23}$$

where $\nu_{\mathrm{L}} = \mu_{\mathrm{L}}/\rho_{\mathrm{L}}$ and $S_{\mathrm{P}} = \rho_{\mathrm{S}}/\rho_{\mathrm{L}}$where U_1, U_2 are the particle settling velocities, ρ_{S}, ρ_{L} are the densities of the particles and the aqueous solution, and μ_{L} is the viscosity (Pa s) of the aqueous solution in the sedimentation unit.

$$Q_0 = F_0\left(1 - \frac{C}{C_{\mathrm{u}}}\right) \tag{24}$$

where F_0 is the input flow rate of the aqueous solution, Q_0 is the over flow rate, C and C_{u} are the concentration of the floc and sludge, and A_{d} is the area of the sedimentation unit:

$$V_{\mathrm{actual}} = \frac{Q_0}{A_{\mathrm{d}}} \quad \text{or} \quad V_{\mathrm{actual}} = F_0\frac{(1 - C/C_{\mathrm{u}})}{A_{\mathrm{d}}} \tag{25}$$

where $A_{\mathrm{d}} = \pi D_{\mathrm{s}}^2/4$ and D_{s} is the diameter of the sedimentation unit.

V_{actual} is actual upward velocity of over flow water.

Check if $V_{\mathrm{actual}} < U_{\mathrm{i}}$, U_{i} means U_1 or U_2

If false, then increment the value of diameter, D_{s} of the sedimentation unit and recalculate V_{actual}.

If true, proceed below to calculate efficiency:

$$\eta = 1 - \left[1 + n\left(\frac{U}{V_{\mathrm{actual}}}\right)\right]^{-1/n}, \qquad n = 0 \text{ or } \frac{1}{8} \text{ or } \frac{1}{4} \text{ or } \frac{1}{2} \text{ or } 1 \tag{26}$$

$V_{\mathrm{desired}} < U.$

2.2.6. Determination of the filtration pressure drops due to filter cake and filter medium

$$\varepsilon = \varepsilon_0(1 - 0.39t^2 - 0.45t) \tag{27}$$

$$L = 0.34t^{0.5} + 0.001 \tag{28}$$

$$V_{\mathrm{F}} = V_0F_0(1 - 0.003Lt) \tag{29}$$

$$(-\Delta P_{\mathrm{c}}) = 180\mu L\frac{V_{\mathrm{F}}(1 - \varepsilon)^2}{\mathrm{d}_{\mathrm{P}}^2\varepsilon^3} \tag{30}$$

$$-\Delta P = (-\Delta P_{\mathrm{c}}) + (-\Delta P_{\mathrm{f}}) \tag{31}$$

where ε is the porosity of the filter cake, L the cake thickness (m) and $-\Delta P_{\mathrm{f}}$ is the pressure drop through the filter medium.

2.3. The overall procedure of computation and output generation

The overall procedure of computation and graphical output generation consists of the following steps:

(i) First a data base is defined that contains initial parameter values.
(ii) Solution of temporal derivatives is done by calling a Runge–Kutta–Fehlberg [16] subroutine using initial value data base.
(iii) Physico-chemical model parameters are computed using standard theoretical correlations or through regression. Among the parameters, the time-dependent parameters are continuously updated in their respective data bases till

convergence. The other time-independent parameters are stored as constants in their respective data bases.

(iv) The initial data base is then updated through step (ii).

(v) Comparison is done in the next step for set error tolerance and steps (i) through (iv) are repeated till convergence.

(vi) The final values of the dependent variables thus obtained are then stored separately in their respective data bases of different units.

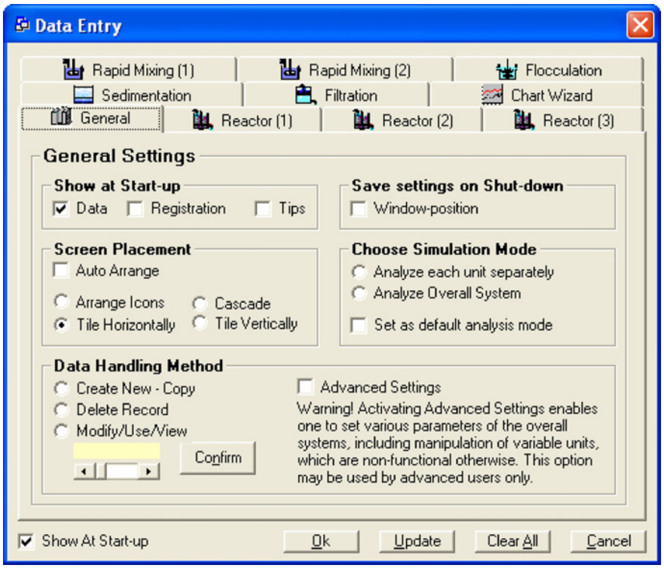
(vii) Desired, preset graphical outputs are then generated using the data bases.

2.4. *The numerical solution scheme and error monitoring*

Other than simple algebraic equations, the model involved a number of coupled ordinary differential equations. For numerical solution of the coupled differential equations, the Runge–Kutta–Fehlberg [16] method was used. The integration procedure incorporated an automatic integration step size adjustment mechanism. The maximum permissible relative error was set at 0.01 and all computations were carried out within this tolerance limit.

3. Software description

The 'ARSEPPA' simulation software has been written in Visual Basic. This is an add-in in Microsoft Excel. The user-friendly menu-driven program is capable of producing the output through visual graphics. The overall process consists of five different units namely; reactor or oxidizer, coagulator or quick-mixing unit, flocculator or slow-mixing unit, a sedimentation unit and a filter unit. One can analyze the performance of the individual units as well as the overall process applying the software. The salient features of data input, data output, method setting, input data updating and screen placement are illustrated through Figs. 1–12.



General Settings

Show at Start-up
☑ Data ☐ Registration ☐ Tips

Save settings on Shut-down
☐ Window-position

Screen Placement
☐ Auto Arrange
○ Arrange Icons ○ Cascade
● Tile Horizontally ○ Tile Vertically

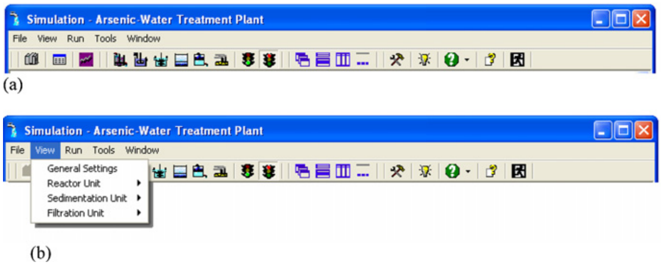
Choose Simulation Mode
○ Analyze each unit separately
○ Analyze Overall System
☐ Set as default analysis mode

Data Handling Method
○ Create New - Copy
○ Delete Record
○ Modify/Use/View

☐ Advanced Settings
Warning! Activating Advanced Settings enables one to set various parameters of the overall systems, including manipulation of variable units, which are non-functional otherwise. This option may be used by advanced users only.

☑ Show At Start-up

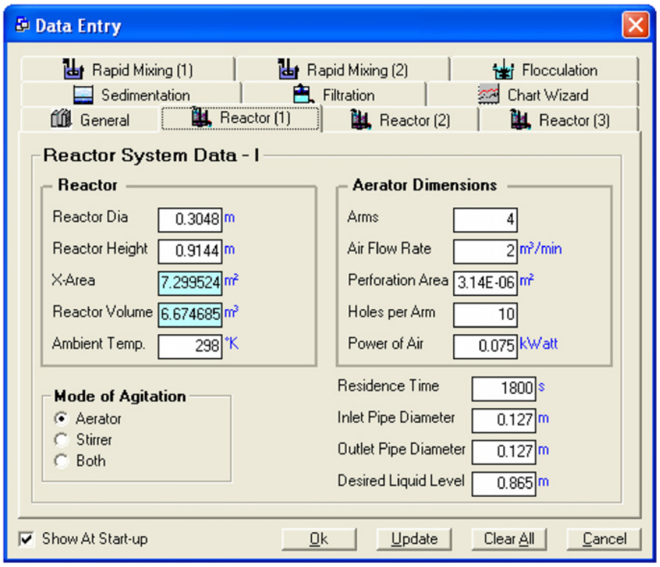
Fig. 1. An interface for general data entry.



(a)

(b)

Fig. 2. The user interface view of the tool bar.



Reactor System Data - I

Reactor
Reactor Dia 0.3048 m
Reactor Height 0.9144 m
X-Area 7.299524 m²
Reactor Volume 6.674685 m³
Ambient Temp. 298 °K

Aerator Dimensions
Arms 4
Air Flow Rate 2 m³/min
Perforation Area 3.14E-06 m²
Holes per Arm 10
Power of Air 0.075 kWatt

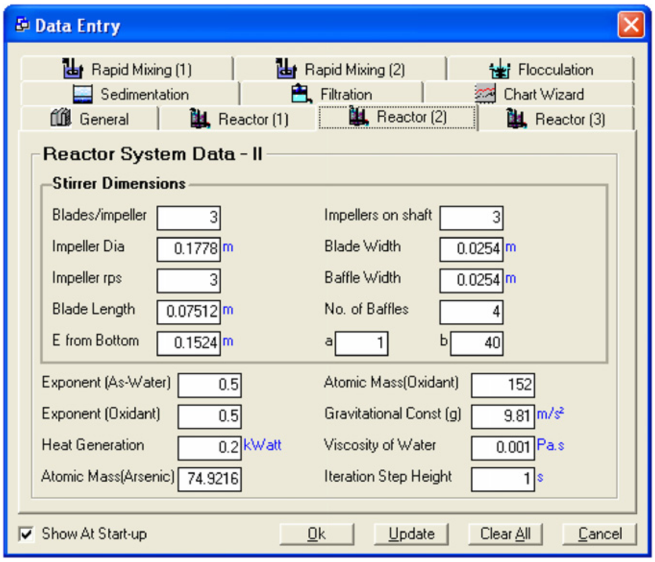
Mode of Agitation
● Aerator
○ Stirrer
○ Both

Residence Time 1800 s
Inlet Pipe Diameter 0.127 m
Outlet Pipe Diameter 0.127 m
Desired Liquid Level 0.865 m

☑ Show At Start-up

Fig. 3. The first input data sheet of the reactor.

The general data sheet as shown in Fig. 1 appears on running the software. It incorporates a user guidance under the '*Show Tips*' option to use the software. The 'Screen *Placement*' option permits visualization of different windows in different styles like '*Tile Cascade*', 'Horizontally,' '*Tile vertically*', etc. The '*Choose*



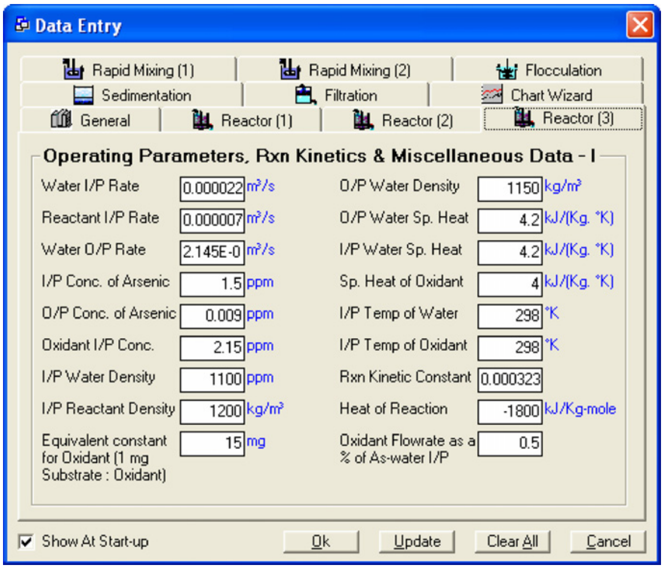
Reactor System Data - II

Stirrer Dimensions
Blades/impeller 3
Impeller Dia 0.1778 m
Impeller rps 3
Blade Length 0.07512 m
E from Bottom 0.1524 m
Impellers on shaft 3
Blade Width 0.0254 m
Baffle Width 0.0254 m
No. of Baffles 4
a 1
b 40

Exponent (As-Water) 0.5
Exponent (Oxidant) 0.5
Heat Generation 0.2 kWatt
Atomic Mass(Arsenic) 74.9216
Atomic Mass(Oxidant) 152
Gravitational Const (g) 9.81 m/s²
Viscosity of Water 0.001 Pa.s
Iteration Step Height 1 s

☑ Show At Start-up

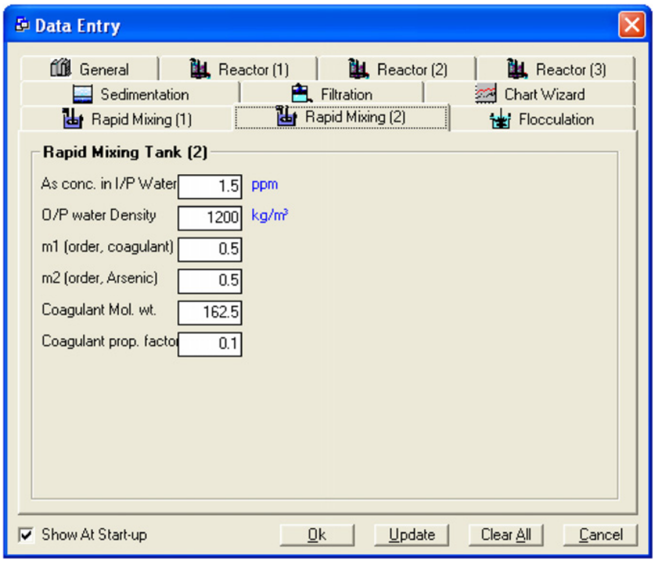
Fig. 4. The second input data sheet of the reactor.



Operating Parameters, Rxn Kinetics & Miscellaneous Data - I

Water I/P Rate: 0.000022 m^3/s
Reactant I/P Rate: 0.000007 m^3/s
Water O/P Rate: 2.145E-0 m^3/s
I/P Conc. of Arsenic: 1.5 ppm
O/P Conc. of Arsenic: 0.009 ppm
Oxidant I/P Conc.: 2.15 ppm
I/P Water Density: 1100 ppm
I/P Reactant Density: 1200 kg/m^3
Equivalent constant for Oxidant (1 mg Substrate : Oxidant): 15 mg
O/P Water Density: 1150 kg/m^3
O/P Water Sp. Heat: 4.2 kJ/(Kg. °K)
I/P Water Sp. Heat: 4.2 kJ/(Kg. °K)
Sp. Heat of Oxidant: 4 kJ/(Kg. °K)
I/P Temp of Water: 298 °K
I/P Temp of Oxidant: 298 °K
Rxn Kinetic Constant: 0.000323
Heat of Reaction: -1800 kJ/Kg-mole
Oxidant Flowrate as a % of As-water I/P: 0.5
☑ Show At Start-up

Fig. 5. The third input data sheet of the reactor.



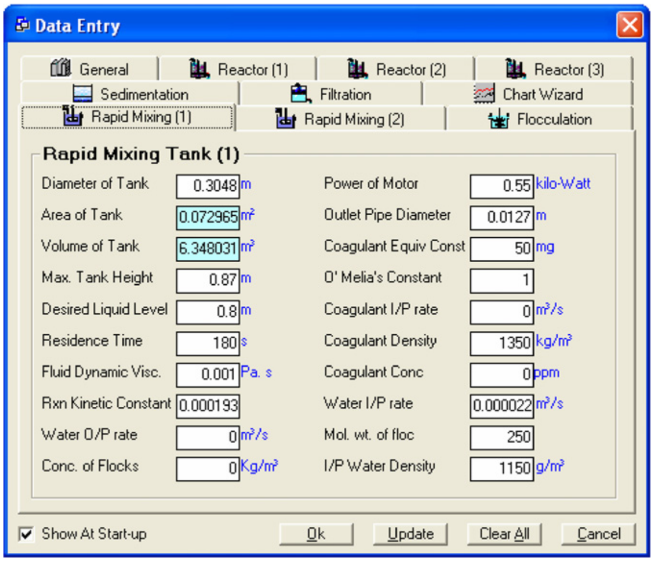
Rapid Mixing Tank (2)

As conc. in I/P Water: 1.5 ppm
O/P water Density: 1200 kg/m^3
m1 (order, coagulant): 0.5
m2 (order, Arsenic): 0.5
Coagulant Mol. wt.: 162.5
Coagulant prop. facto: 0.1
☑ Show At Start-up

Fig. 7. The second input data sheet of the Quick mixing tank (coagulator).

Simulation Mode' option permits performance analysis of either individual units or the overall process as a whole. The '*Data Handling Method*' option incorporates the provision for setting the parameters of the input data sheet. Unless a new method is set up, the simulation runs by default using the set parameters. The 'View' tab permits checking of the saved data sheets under specified data sheet number. '*Clear All*' tab helps to rewrite new data sheet on erasing the existing one. 'Update' tab saves the newly created data sheet.

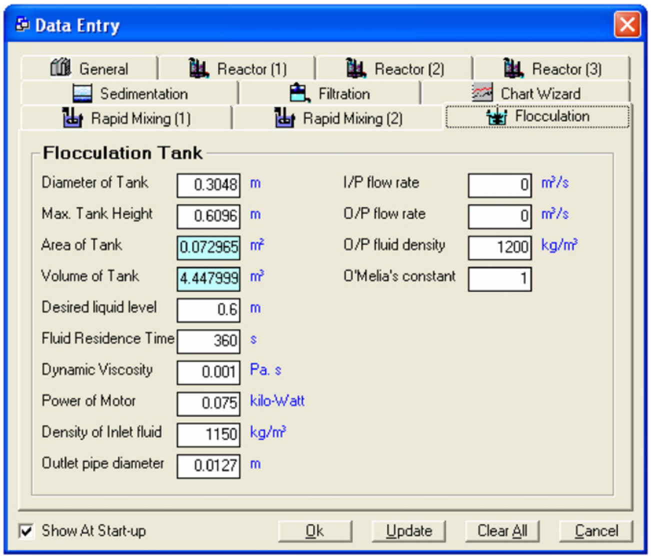
Fig. 2(a) and (b) shows the main window tool bar. The tool bar contains the icons of all the units', viz., reactor, quick mixing unit, slow mixing unit, sedimentation unit and the filtration unit. The tool bar provides for two separate tabs, namely, 'Start *Simulation*' and 'Stop *Simulation*'. To run the simulation one has to select the desired unit and then click on the 'Start *Simulation*'. Simulation results are displayed graphically. One can get the results sheet also selecting 'Grid *Data*' menu. Graphical simulation results are obtained both in multi-window fashion as well as in cascade style. Using the appropriate tools of the chart sheet tool bar, out puts can be printed or saved. The tool bar incorporates facility of graph editing. The grid data values can be directly transferred to Excel sheet for generating secondary graph sheets. To analyze the overall system for performance one has to select the 'Run' tab first then, 'Overall *System*' option and 'Start *Simulation*' option sequentially. The tool bar also has the provision for file handling under the name 'Disk *Utility Station*'. One can create or remove a folder and delete or move a file using the tool. From the *File* tab one can open new run sheet or an old saved sheet. The tab also includes functions like print, preview etc. In *Tools* tab, different tools like '*Export data sheet*' to Excel sheet or vice versa are there.



Rapid Mixing Tank (1)

Diameter of Tank: 0.3048 m
Area of Tank: 0.072965 m^2
Volume of Tank: 6.348031 m^3
Max. Tank Height: 0.87 m
Desired Liquid Level: 0.8 m
Residence Time: 180 s
Fluid Dynamic Visc.: 0.001 Pa. s
Rxn Kinetic Constant: 0.000193
Water O/P rate: 0 m^3/s
Conc. of Flocks: 0 Kg/m^3
Power of Motor: 0.55 kilo-Watt
Outlet Pipe Diameter: 0.0127 m
Coagulant Equiv Const: 50 mg
O' Melia's Constant: 1
Coagulant I/P rate: 0 m^3/s
Coagulant Density: 1350 kg/m^3
Coagulant Conc: 0 ppm
Water I/P rate: 0.000022 m^3/s
Mol. wt. of floc: 250
I/P Water Density: 1150 g/m^3
☑ Show At Start-up

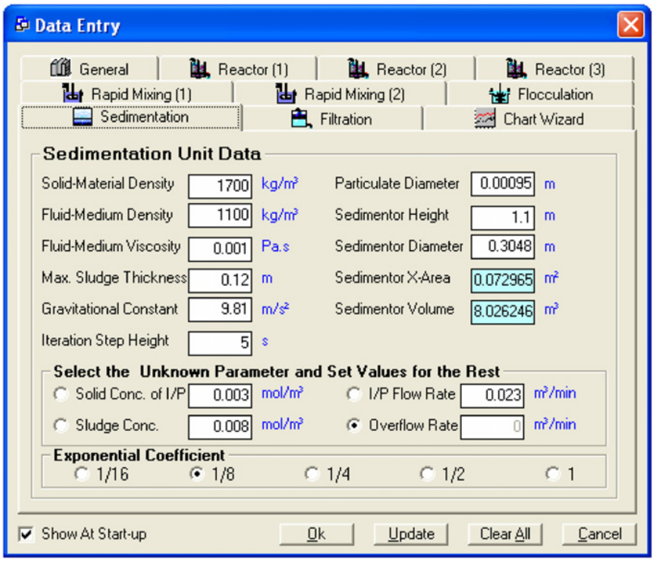
Fig. 6. The first input data sheet of the Quick mixing tank (coagulator).



Flocculation Tank

Diameter of Tank: 0.3048 m
Max. Tank Height: 0.6096 m
Area of Tank: 0.072965 m^2
Volume of Tank: 4.447999 m^3
Desired liquid level: 0.6 m
Fluid Residence Time: 360 s
Dynamic Viscosity: 0.001 Pa. s
Power of Motor: 0.075 kilo-Watt
Density of Inlet fluid: 1150 kg/m^3
Outlet pipe diameter: 0.0127 m
I/P flow rate: 0 m^3/s
O/P flow rate: 0 m^3/s
O/P fluid density: 1200 kg/m^3
O'Melia's constant: 1
☑ Show At Start-up

Fig. 8. The input data sheet of the slow mixing tank (flocculator).



Sedimentation Unit Data

Solid-Material Density 1700 kg/m³
Fluid-Medium Density 1100 kg/m³
Fluid-Medium Viscosity 0.001 Pa.s
Max. Sludge Thickness 0.12 m
Gravitational Constant 9.81 m/s²
Iteration Step Height 5 s
Particulate Diameter 0.00095 m
Sedimentor Height 1.1 m
Sedimentor Diameter 0.3048 m
Sedimentor X-Area 0.072965 m²
Sedimentor Volume 8.026246 m³

Select the Unknown Parameter and Set Values for the Rest

○ Solid Conc. of I/P 0.003 mol/m³
○ I/P Flow Rate 0.023 m³/min
○ Sludge Conc. 0.008 mol/m³
● Overflow Rate 0 m³/min

Exponential Coefficient

○ 1/16 ● 1/8 ○ 1/4 ○ 1/2 ○ 1

☑ Show At Start-up

Fig. 9. The input data sheet of the sedimentation unit.

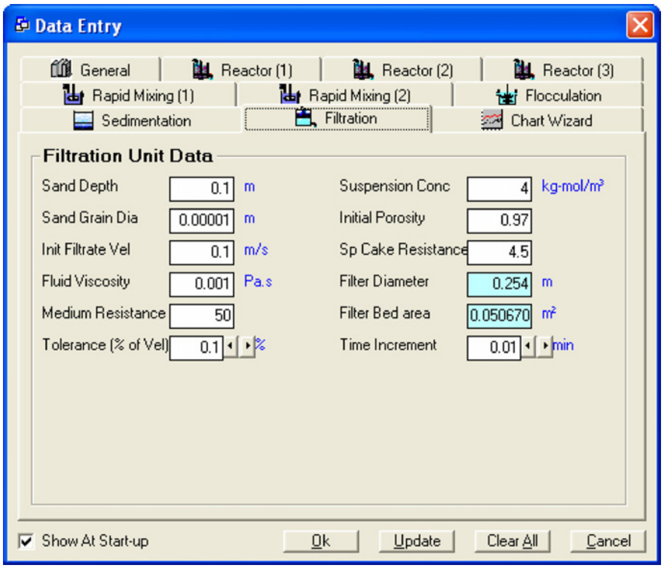
3.1. Software input

The input data required to run the software consists of physical dimensions of each unit and its auxiliary provisions (like stirrer, etc.), kinetic data, operating parameters and physico-chemical data. Under each unit, the relevant data are entered in the preset item boxes. To save the entered data the '*Update*' tab is used. The '*Data Entry*' window has provision for entering the data in different units. Editing of the units can be easily done by pressing the 'U' tab that appears on clicking the data boxes.

Figs. 3–5 show the data entry pattern for the reactor.

Figs. 6 and 7 exhibit how data are entered for the quick-mixing unit.

Figs. 8–10 show the data entry patterns for the slow-mixing unit, the sedimentation unit and the filtration unit, respectively.



Filtration Unit Data

Sand Depth 0.1 m
Sand Grain Dia 0.00001 m
Init Filtrate Vel 0.1 m/s
Fluid Viscosity 0.001 Pa.s
Medium Resistance 50
Tolerance (% of Vel) 0.1 %
Suspension Conc 4 kg-mol/m³
Initial Porosity 0.97
Sp Cake Resistance 4.5
Filter Diameter 0.254 m
Filter Bed area 0.050670 m²
Time Increment 0.01 min

☑ Show At Start-up

Fig. 10. The input data sheet of the filter unit.

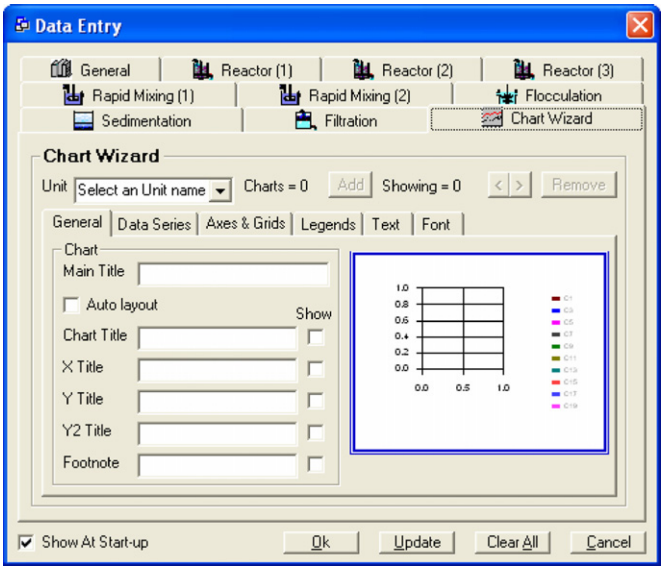


Chart Wizard

Unit Select an Unit name
Charts = 0
Showing = 0

Main Title
☐ Auto layout
Chart Title ☐
X Title ☐
Y Title ☐
Y2 Title ☐
Footnote ☐

☑ Show At Start-up

Fig. 11. Chart wizard is used to see the performance of the different units.

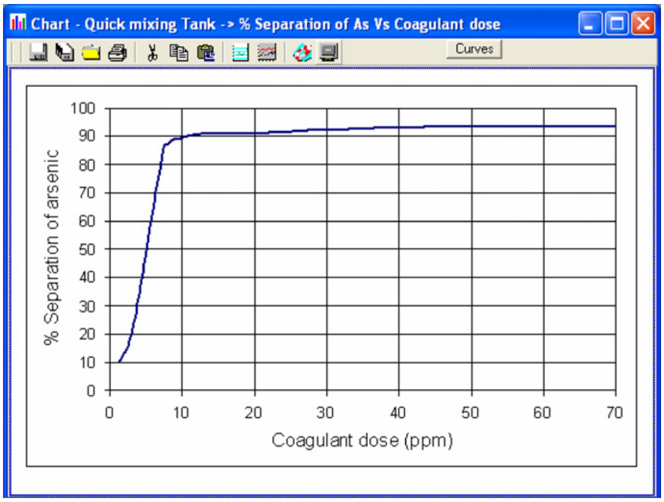


Fig. 12. The output graph sheet generated from program showing the effect of the coagulant dose.

3.2. Software output

Some of the output forms are shown in Figs. 12 and 13.

How the outputs are generated on running the simulation software has been described in Section 2.3. Fig. 11 exhibits how the software-predicted overall performance in terms of % separation of arsenic varies with the experimental findings as a major operating variable coagulant dose changes. A similar performance characteristic curve in Fig. 12 shows the effect of oxidant dose.

4. Software validation

The software was validated by carrying out experimental investigation and comparing the experimental data with the software-predicted values. Some of the graphical comparisons are presented in Figs. 14–17. A typical set of experimental con-

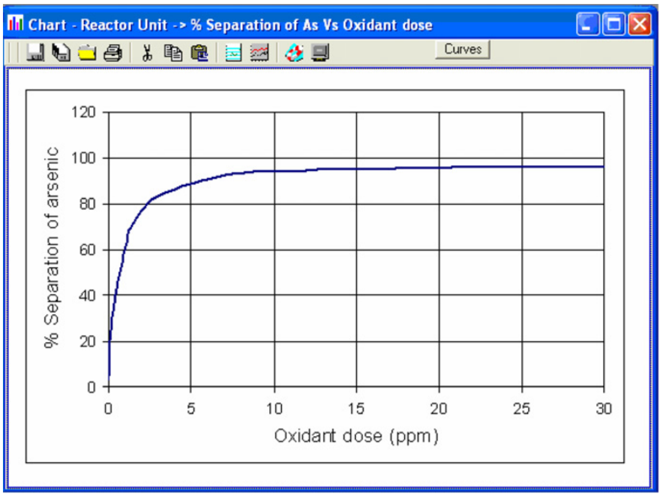


Fig. 13. The output graph sheet generated from program showing the effect of the oxidant dose.

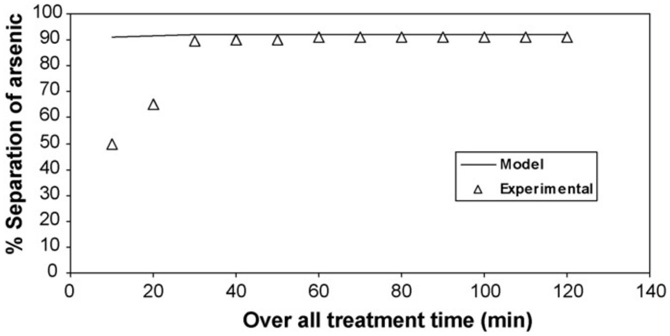


Fig. 14. Overall concentration (in % separation) profile of arsenic in treated water. Experimental conditions: oxidant ($KMnO_4$) conc. 15 ppm; coagulant ($FeCl_3$) conc. 30 ppm; arsenic conc. of feed water 1.0 ppm; feed rate 0.022×10^{-3} m^3/s; pH 7.6; temperature = 305 K. Other conditions are as in Table 1.

ditions under which the investigations were carried out has been presented in Table 1.

Software-predicted arsenic concentration profile of treated water as depicted in Fig. 14 shows around 91–92% removal of arsenic from aqueous phase at steady state. Over an initial period of 30 min, experimental values were far below the model predicted values. This wide deviation was attributable to the unsteady state of the whole plant during this phase. The deviation, however, was gradually smoothed out and the experimental findings were observed to corroborate well with the model predictions. The over all correlation coefficient was found to be 0.98890. The model assumes separation of arsenic basically through enmeshment and adsorption of arsenic onto the metal hydroxides but other mechanisms like formation of precipitates, co-precipitates and mixed precipitates might also be active during the initial unsteady phase resulting in a separation higher than model-predicted ones after the system attains steady state as shown in the figure.

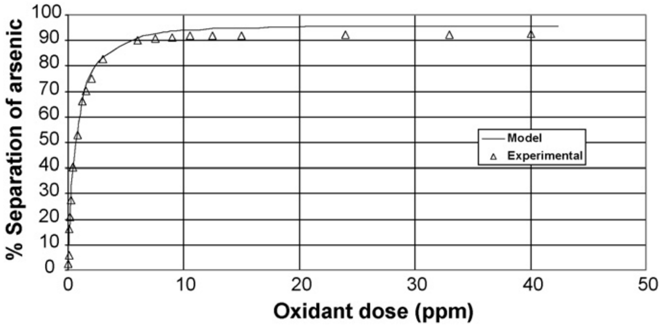


Fig. 15. Effect of oxidant concentration on % removal of arsenic. Experimental conditions: oxidant $KMnO_4$; coagulant ($FeCl_3$) conc. 30 ppm; arsenic conc. of feed water 1.0 ppm; feed rate (m^3/s) 0.022×10^{-3}; pH in the oxidation unit 5.5; pH in the coagulator 7.6; temperature = 305 K.

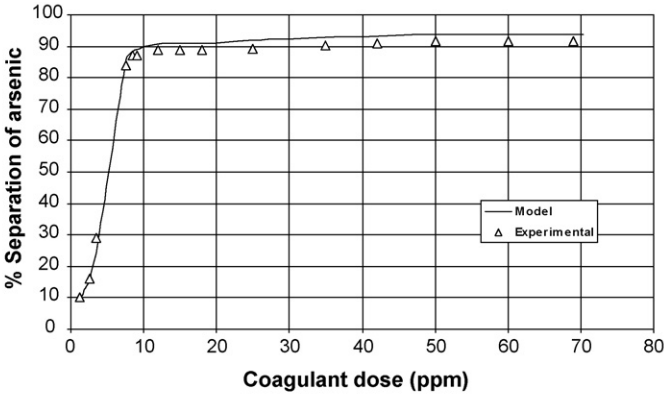


Fig. 16. Effect of ARSEPPA: a Visual Basic Software Tool for arsenic separation plant performance analysis.

Close agreement of the software predictions with the experimental findings only suggests that the model assumptions are largely correct.

Software predictions were also compared with experimental findings while studying the effects of major operating variables like oxidant dose, coagulant dose and feed concentration etc. as presented in Figs. 15–17, respectively. Comparison establishes that though at the lower concentration ranges of oxidant and coagulant doses, deviations between the experimental findings and the software predictions are observed, overall agreement of the software predictions with experimental findings (including

Table 1
Typical set of experimental conditions and model parameters

Experimental conditions/parameters	Values (SI)
Temperature maintained in the units	298–305 K
Root mean square velocity gradient in the coagulator (G_1)	$800\ s^{-1}$
Root mean square velocity gradient in the flocculator (G_2)	$70\ s^{-1}$
Feed water flow rate	$0.022 \times 10^{-3}\ m^3/s$
Arsenic concentration of the feed water	$1–2 \times 10^{-33}\ kg/m^3$
Oxidation rate constant	$3.23 \times 10^{-33}\ s^{-1}$
pH in the oxidation unit	5.5
pH in coagulator and flocculator	7–8
Overall settling rate constant	$1.93 \times 10^{-33}\ s^{-1}$
Coagulant concentration	$30 \times 10^{-33}\ kg/m^3$
Oxidant concentration	$15 \times 10^{-33}\ kg/m^3$

feed concentration effects) is reasonably good. This establishes capability of the software in analyzing performance of an arsenic separation plant with reasonable accuracy.

5. Conclusion

In the present work, a simulation software ('ARSEPPA') written in Visual Basic has been developed for arsenic separation plant performance analysis in the backdrop of absence of such a software. This user-friendly, menu-driven software works in Microsoft Excel environment thereby eliminating the need for familiarity with a new working environment. The software is based on dynamic mathematical model of the systematically integrated physical and chemical processes involved in separation of arsenic from drinking water. Though research abounds physico-chemical separation of arsenic, no simulation package considering the most relevant treatment scheme with the best found chemical reagents has yet been developed. The present work fills up this vacuum through systematically integrating the most relevant physico-chemical processes and developing a dynamic mathematical model of the whole separation scheme. The software has been validated by carrying out detailed experimental investigation and comparing the experimental findings with the model-predicted values. The overall correlation coefficient was found to be of the order of 0.98890. The scheme is successful in achieving a separation efficiency of around 90–92%. Though higher efficiency achievement has been reported in the literature [11,12] for batch processes, an efficiency of 90–92% may be considered quite high for a continuous process of the present study. So the software deals with a continuous process achieving high efficiency. One can observe the effects of all the major operating variables on the performance of the overall system as well as the individual units that are integrated into the scheme. This in turn allows optimization of the operating variables under different situations. The software permits pre-analysis manipulation of the input data and graphical visualization of the output in a familiar environment. Though developed for arsenic separation plant performance analysis, the software can well be extended to separation of many other heavy metals like calcium, magnesium, cadmium, lead, etc. The software is expected to be extremely useful in raising the level of confidence in designing and operating physico-chemical treatment plants for separation of arsenic from drinking water.

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