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## Visualizing Solubilization by a Realistic Particle Model in Chemistry Education

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**Abstract.** An application for the visualization of the mixing process of two different types of structureless interacting particles is presented. The application allows to demonstrate on a qualitative basis, as well as by quantitatively monitoring the time evolution of the fractions of aggregates of different sizes, that the formation of a homogeneous mixture is the result of favorable solute-solvent interactions as well as by temperature. It is suggested that, along with the use of suitable macroscopic examples, visualizations by the present application are useful in elucidating concepts related to miscibility/solubility. The application is based on a two-dimensional realistic dynamic model where atoms move because of their thermal and interaction potential energies and their trajectories are determined by solving numerically Newton's laws according to a Molecular Dynamics (MD) scheme. For this purpose, a web-based MD engine was adapted as needed. It is suggested that, when possible, using a realistic simulation rather than simple animations offers several advantages in the visualization of processes of interest in chemistry education. First of all, in a simulation the outcome of the process under study is not set *a priori* but it is the result of the dynamic evolution of the system; furthermore, specific parameters can be systematically varied and the effects of these changes can be investigated. The application can be used at different levels of detail and in different instruction levels. Qualitative visual observations of the obtained mixtures are suitable at all levels of instruction. Systematic investigations on the effect of changes in temperature and interaction parameters, suitable for senior high school and college courses, are also reported.

**Keywords.** Chemistry Education, Intermolecular Interaction, Mixtures, Molecular Dynamics, Particle Model, Solubility.

### INTRODUCTION

The particle model of matter has been extensively used in the past to interpret and visualize different kinds of chemistry processes and phenomena for education purposes also pointing out its shortcomings as a potential source of misconceptions<sup>1-15</sup>{Johnstone, 1991 #1}.

An effective way of introducing the particle model of matter, in our opinion, is to quote a quite famous sentence<sup>16</sup> by Richard Feynman (1918-1988), Nobel laureate in physics in 1965:

*If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generations of creatures, what statement would contain the most information in the fewest words? I believe it is the atomic hypothesis (or the atomic fact, or whatever you wish to call it) that all things are made of atoms—little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another. In that one sentence, you will see, there is an enormous amount of information about the world, if just a little imagination and thinking are applied.*

The above sentence suggests that the main ingredients to be stressed and clarified are: existence of discrete particles, motion and interactions. These concepts are equally important and they must be all present in any exhaustive implementation of the particle model for education purposes but they should be introduced gradually in a process of progressive development of the model inspired by the comparison between its predictions and experimental evidences.

In particular, when only still pictures are used, the dynamic properties of matter are inevitably lost in spite of the fact that they are as important as structural considerations in determining the system overall behavior. This is important for physical properties, where no changes in chemical identity of the particles are involved, as well as for chemical transformations.

Due to the continuing progress in computing power and in modelling software, in addition to advanced tools for the visualization of molecular structures, many different dynamic visualization tools have become readily available, either on the web or stand-alone, even for popular devices such as tablets and smartphones<sup>17-23</sup>.

However, in most animations<sup>22, 24-29</sup>, particle motion is defined in a more or less arbitrary way. Realistic dynamic models are seldom used for education purposes<sup>30-35</sup>. A computer application for the visualization of the aggregation and growth process of nanoparticles by a Molecular Dynamics (MD) realistic model has been recently presented<sup>36</sup>. In the same study, the advantages of adopting, when possible, a molecular simulation perspective rather than using simple animations have been discussed.

In this work, we preset an application, based on the same realistic model, designed to introduce a progressive development of the particle model for visualization and education objectives. The application was specifically implemented for elucidating solubility, i.e. the phase behavior of a two-components mixture of different particles. After a brief summary of the Molecular Dynamics (MD) method, the application is discussed by following

a step-by-step sequence leading to its final objective.

## THE MOLECULAR DYNAMICS METHOD

In the MD simulation method, a fixed number of atoms/molecules move in a given volume and behave as classical objects. Their motion is the consequence of both thermal and interaction potential energies. The particle motion is ruled by Newton's classical laws:

$$m_i \ddot{\mathbf{r}}_i = -\nabla_i(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \quad (1)$$

where  $\mathbf{r}_i$  is the position vector of the  $i$ -th atom and  $m_i$  is its mass. Hence, in order to calculate the trajectory of each atom, one needs to solve numerically 3 second order differential equations for each time step  $dt$ . As a consequence, for the design of an MD simulation, substantial computing and programming abilities are required. However, as already pointed out<sup>36</sup> and as done in the present work, an efficient and easy to use web-based resource<sup>37</sup> can be used.

The interested reader can find full details about MD elsewhere<sup>31, 38-40</sup>. In what follows, we will limit the discussion to the dynamic description of a set of  $N$  interacting structureless atoms.

In the case under consideration, an appropriate form of the interaction energy is given by the so-called Lennard-Jones (LJ) potential:

$$U_{i,j, i \neq j} = 4\epsilon \cdot \left[ \left( \frac{\sigma}{R_{ij}} \right)^{12} - \left( \frac{\sigma}{R_{ij}} \right)^6 \right] \quad (2)$$

$$U = \frac{1}{2} \cdot \sum_{i,j, i \neq j} U_{i,j} \quad (3)$$

where  $R_{ij}$  is the distance between the  $i$ -th and  $j$ -th atom,  $\epsilon$  is a parameter related to the attractive strength and  $\sigma$  is the atomic diameter corresponding to the contact distance. As a consequence, the total potential energy is calculated as the sum of all pairwise contributions defined by Equation 2. In this equation, the first term, sharply increasing with decreasing interparticle distance, is attributable to repulsions at contact distances whereas the negative term represents long-range attractions.

In order to start an MD simulation, one has to define initial positions and velocities of each particle. A common choice is to place the  $N$  particles in random positions of the simulation cell with a velocity distribution close to that given by the Maxwell-Boltzmann particle distribution<sup>41</sup>:

$$f(v) = 4\pi \left( \frac{m_i}{2\pi k_B T} \right)^{3/2} v_i^2 \exp\left( -\frac{m_i v_i^2}{2k_B T} \right) \quad (4)$$

where  $f(v)$  is the probability distribution of speed,  $m_i$  and  $v_i$  are the mass and the component of the velocity of the  $i$ -th atom,  $T$  is the temperature,  $k_B$  is Boltzmann's constant.

The MD procedure consists in solving Equation 1 for each atom at a given time step and iterating for successive discrete time steps, thereby producing a time sequence of configurations.

#### PARTICLE MODEL IMPLEMENTATION

In this work, we present a computer application<sup>42</sup> which uses Molecular Workbench (MW), an open-access web-based general purpose MD engine developed by the Concord Consortium<sup>37</sup>. This Java based platform provides 2D and 3D classical molecular dynamics engines. In addition to ready-made examples, the user can design and customize new models or activities. Full details about the computation environment are given elsewhere<sup>35</sup>.

In the use of the application, the first step is to illustrate the opening sentence in Feynman's statement mentioned in the Introduction: *things are made of atoms—little particles that move around in perpetual motion*.

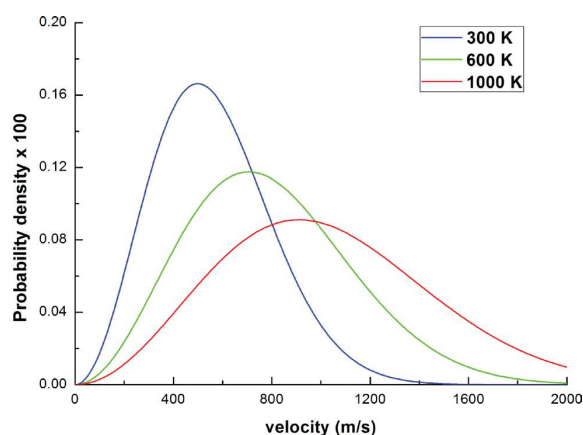
When the application is first started, at the top of the page, the user is presented with an empty container: a  $100 \times 100 \times 100 \text{ \AA}^3$  cell. An arbitrary number  $N$  ( $0 \leq N \leq 500$ ) of identical monoatomic structureless particles with diameter  $\sigma = 2.0 \text{ \AA}$  and mass  $m = 20 \text{ gmol}^{-1}$ , can be placed in random positions of the simulation cell by clicking on the appropriate control after selecting the desired number of particles. It is important to specify that these particles behave as tiny hard spheres and, as a consequence, their shape and size cannot change. After selecting the desired value of the temperature ( $100 \leq T \leq 1000$ ), by clicking on the "Run the model" button, the simulation will start and the particles will move by following Newton's laws of motion and undergoing virtually elastic collisions among them. In this case, no long-range attractive interactions were set, i.e. the  $\epsilon$  value in Equation 2 was set to a very small value ( $\epsilon = 0.01 \text{ eV}$ ). As a consequence, it can be easily observed that, between collisions, particle motion is unaffected by the presence of the other particles. Students should be encouraged to observe and describe the behavior of the system and, if desired, the instructor may ask appropriate questions in order to assess students' understanding. For example, in lower secondary school classes, students might be asked to suggest the nature of the medium in which the particles are moving or whether there might be a tangible consequence of the particle collisions on the container walls. At this stage, other possible qualita-

tive observations that the instructor might consider to initiate, deal with the effect of changing the temperature on particles velocities and/or that of changing the number of particles in the given (fixed) volume on the empty space available to the particles. This latter concept is connected to those of compressibility and density of gases. The instructor will decide the level of the discussion based on the students' background. It is important to stress that, in this preliminary phase, students should be mainly asked to observe the phenomena on their own and address possible problematic situations appropriately proposed by the instructor.

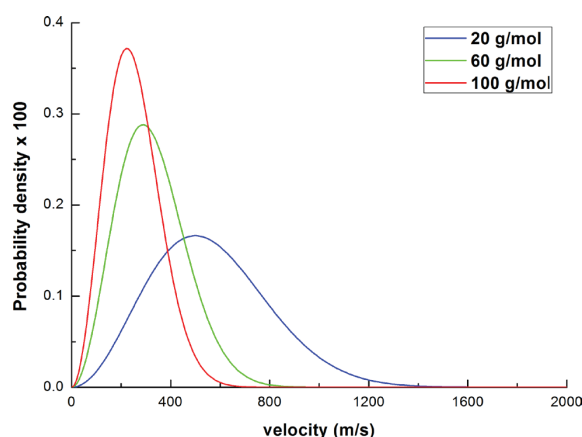
From now on, all further demonstrations by the current application will be implemented in a 2D environment. This choice is justified by the fact that the application should be run interactively and students should be put in the position to observe significant results in a reasonable time. In an MD simulation, the most time-consuming step is the double loop (see Equation 3) in which the interactions between each particle and its neighbors are calculated. The number of terms to be calculated scales roughly as  $N^2$ . As a consequence, computing time increases quadratically with  $N$ . For this reason, it is important to keep the number of atoms  $N$  as small as possible. By adopting a 2D environment, it is possible to reduce drastically the number of particles to be included in the simulation without any significant loss in physical realism, at least for the phenomena and concepts here considered.

In the application, the second demonstration, at the bottom of the page, is designed to study in more detail a few of the concepts already introduced. In particular, in addition to their number, the size and mass of the atoms can be changed within specified ranges. Different particle colors are used when their mass is changed, in order to indicate that the type of particles has changed. At this point, a definition of *substance* at the submicroscopic level can be introduced as a portion of matter constituted by identical particles. Particles of a given substance, then, are identical but they are different from those of a different substance. Thus, a mixture of different substances contains particles of different types. It might be objected that a mass change without a corresponding change in atomic size is unlikely. However, at this stage, it was chosen not to stress the correspondence between atomic properties and their chemical identity. In our opinion, this correspondence will come into play later when elements and periodicity will be introduced.

Once again, in introductory science/chemistry instruction (upper primary and lower secondary school classes), effects due to changes in atomic properties (size and mass) and temperature can be investigated on a



**Figure 1.** Maxwell-Boltzmann probability distribution of atomic velocities (see Eq. 4) at the temperatures specified in the legend for a set of 200 atoms of mass  $m = 20$  g/mol. The MD time step was 1 fs.



**Figure 2.** Maxwell-Boltzmann probability distribution of atomic velocities (see Eq. 4) at  $T = 300$  K for a set of 200 atoms with mass  $m$  specified in the legend. The MD time step was 1 fs.

qualitative basis. In upper high school and introductory university courses, a more quantitative approach can be adopted. In this part of the application, it is possible, for example, to calculate the Maxwell-Boltzmann (see Equation 4) speed and velocity distributions. It might be recalled that the difference between the two functions is that, in the former case, one considers a scalar quantity, i.e. the module of the velocity vector.

In Figures 1 and 2, results obtained with the specified parameters demonstrate that the most probable atomic speed increases with increasing temperature and decreasing atomic mass. This evidence illustrates the connection between temperature and the average kinetic energy of the atoms. The instructor will be able to tune the level of this description to the students' background even recalling basic concepts about the laws of motion as needed.

The corresponding velocity distribution function that can be calculated by activating the appropriate button in the application, will exhibit a maximum at  $v \approx 0$  indicating that, since atoms are moving in all directions, there is no net resulting component of the velocity vector.

At this point of the teaching sequence, interactions among particles can be introduced. Going back to Feynman's quote:

*...attracting each other when they are a little distance apart, but repelling upon being squeezed into one another.*

Therefore, the interaction energy is negative (attractive) when atoms are at intermediate distances and it becomes positive (repulsive) when they get close to each other. When interatomic average distances are large, the

interaction potential approaches zero. For the case under consideration here, a convenient form of the interaction potential is that given by Equation 2.

The introduction of interactions and the balance with atomic average kinetic energy leads to discussions related to physical states of matter, in particular the existence of condensed (solid and liquid) phases and phase transformations. This topic is not part of the present work and it will not be discussed further. However, many different dynamic applications can be found in the literature. In particular, an explicit connection between interactions, particle motion and phase behavior is available in a recent study<sup>36</sup> as well as ready-made examples in the MW website<sup>43, 44</sup>.

## MIXTURES AND SOLUBILITY

The concept of solubility is one of the most common themes in chemistry and, at the same time one of the most difficult to grasp by students on a conceptual basis. Anyone is familiar with the macroscopic difference between a solution, such as the result of the addition of a not too large amount of sodium chloride to water, and the result obtained by mixing olive oil and water. However, things get complicated when rigorous definitions are sought. These definitions, on the macroscopic level, essentially involve the concept of *phase* and, thus, a homogeneous mixture (a solution), consists of a single phase whereas, in a heterogeneous mixture, at least to different phases can be detected. On the submicroscopic scale, in spite of its potential conceptual hurdles, the particle model offers, in our opinion, a more logical

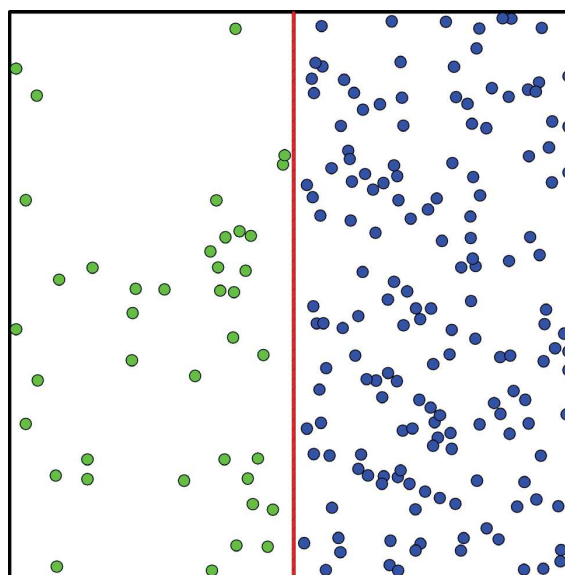
representation, particularly when the dynamics are also taken into account. In this perspective, in a mixture of particles of type A and type B, a phase is recognizable as a cluster of B particles dispersed within A particles. Incidentally, a system containing different phases of the same substance, such as ice floating in liquid water, can be described as clusters of particles of a given type in a given structure within particles of the same type in a different structure.

The factors affecting the stability of a mixture of two different substances and determining solubility/miscibility can be rationalized by analyzing the thermodynamics of the mixing process<sup>45, 46</sup>. This topic has been also the object of many studies for education purposes<sup>47-52</sup>. In short, entropy always favors mixing whereas reciprocal particle interactions between like and unlike species can influence the process in both directions. In addition, temperature plays a role in that, in most cases, the mixing of simple systems is favored by an increase in the temperature.

All the above ideas have been gathered in the second page of the present application. This page also contains a link to a brief section on general background concepts. When the application is first started, the user is presented with an empty container: a 60 x 60 Å<sup>2</sup> cell. A barrier divides the cell into two compartments where a specified number of equally sized ( $\sigma = 1.4$  Å) A (blue) and B (green) particles of the same mass ( $m = 40$  gmol<sup>-1</sup>) can be placed. The user selects the total number of atoms  $N$  ( $50 \leq N \leq 200$ ) and the fraction (0-0.5) of B atoms. When this is done, the specified number of B atoms is placed, in random positions, on the left hand side of the barrier; the number of A atoms, resulting from the specified B fraction, is placed, in random positions, on the right hand side of the barrier. In Figure 3, a typical configuration of a sample simulation with the specified parameters is shown.

Furthermore, the strength,  $\epsilon$  (eV) of the attractive part of the LJ potential (see Equation 2) between all particles will have to be set. The user can set independently the strength of the potential between A particles ( $\epsilon_{A-A}$ ), between B particles ( $\epsilon_{B-B}$ ) and between A and B particles ( $\epsilon_{A-B}$ ). Finally, a specific control allows to set the temperature  $T$  of the simulation. When all parameters have been selected, the simulation will start by clicking on the "Run the model" button. By clicking on the "Mix" button, the gate between the two compartments opens and the two groups of particles mix.

During the simulation, the plot on the right will display the time evolution of the fractions, with respect to the total number of B particles present as B monomers, B pairs and B atoms present in larger aggregates. In this



**Figure 3.** Initial configuration of a mixture of A (blue) and B (green) structureless equally sized ( $\sigma = 1.4$  Å) particles in a 60x60 Å<sup>2</sup> simulation cell. The total number  $N$  of particles was 200 and the fraction of B particles was 0.2. At the beginning of the simulation, A and B particles are contained in two compartments separated by the impermeable barrier also shown.

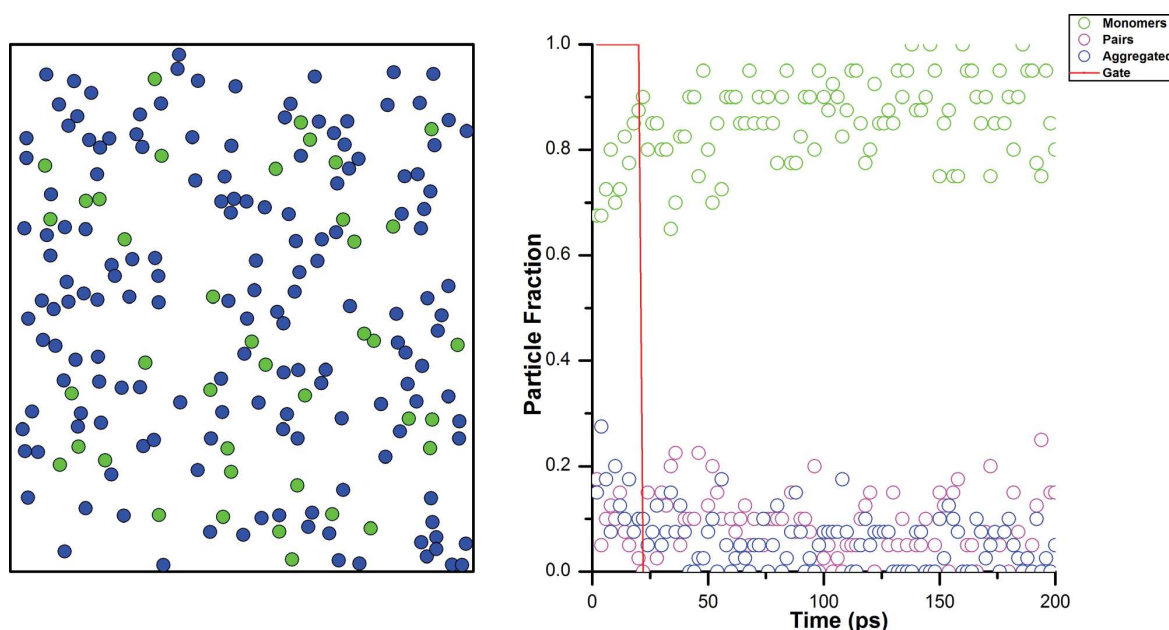
plot, the red line, initially set at a value of 1, drops to 0 when the gate is opened.

In Figure 4, results of a sample simulation performed with the specified parameters are shown. It can be seen that, when all interaction parameters are very small ( $\epsilon \approx 0$  eV), the driving force to mixing is entropy and a homogeneous distribution of B particles in the A solvent is quickly obtained.

By running the simulation at different thermal conditions, it is easy to prove that temperature influences the rate of the mixing progress but not its outcome.

In Figure 5, results from a simulation performed with parameters favoring B-B interactions are shown. It can be seen that, after the barrier is removed, the substances mix but, because of preferential B-B interactions, the solute is present as aggregates of different sizes within the A matrix.

By prolonging the simulation, it can be observed that B clusters tend to merge with each other forming larger aggregates, thereby maximizing B-B contacts and minimizing energy. In this case, a heterogeneous mixture of B in A is obtained. The same qualitative conclusions are obtainable from the plot on the right of the same figure: a progressive decrease in the fraction of B monomers corresponds to an increase of the fraction of B aggregates.



**Figure 4.** Left: snapshot of the configuration obtained after 200 ps of a simulation for the mixture described in Figure 3 at  $T = 300$  K and no interactions between the particles. Right: time evolution of the fraction of B monomers, pairs of B atoms and total aggregated B atoms present in clusters of more than 2 B atoms for the same simulation. The time at which the red line sharply drops to zero indicates when the gate shown in Figure 3 was opened and the particles were allowed to mix. The MD time step was 1 fs.

On the contrary, as shown in Figure 6, by adopting conditions favoring A-B interactions a homogeneous dispersion of B in A is quickly obtained. The plot on the right demonstrates that the vast majority of B atoms is present as monomers; a few pairs and slightly larger aggregates are also present.

The effect of temperature is demonstrated in Figure 7. In this case, the heterogeneous mixture obtained under the conditions of Figure 6, was heated to two different temperatures. Heating favors the formation of a homogeneous system as shown by the progressive “melting” of the B aggregates.

This conclusion is supported by the plot on the right showing a progressive increase in the fraction of B monomers at the expense of large B aggregates.

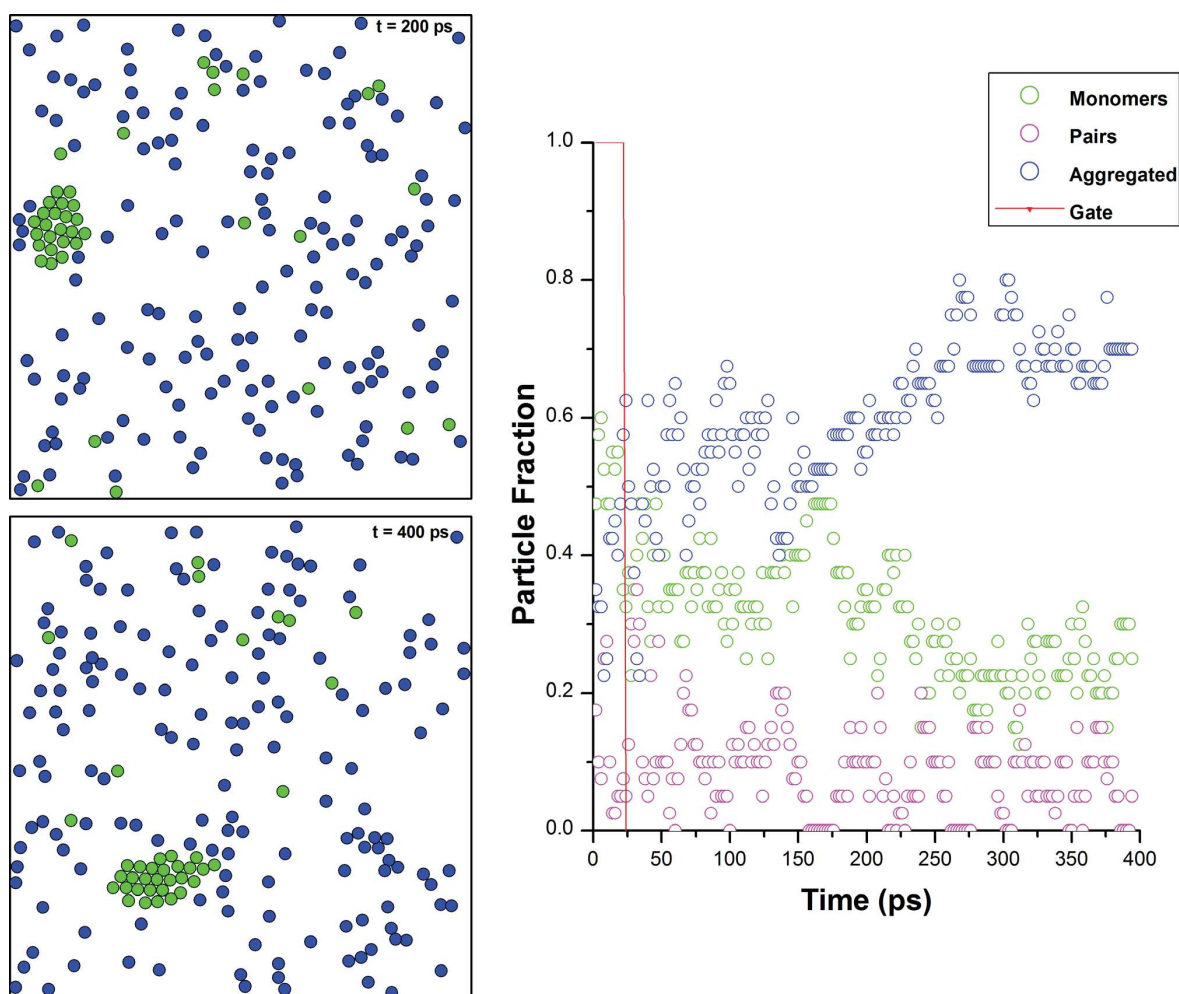
As an additional evidence in support of the previous conclusion, in Figure 8 results obtained at  $T = 500$  K from a simulation started from an initial configuration similar to that of Figure 3 are shown. At this temperature, contrary to what observed at  $T = 300$  K (see Figure 5), a homogeneous B in A mixture is obtained.

In the plot on the right, it is demonstrated on a quantitative basis that, throughout the simulation, the vast majority of B atoms is present as monomers.

## DISCUSSION

The present application has been designed to introduce the basic concepts of the particle model of matter and, in particular, its dynamic properties. It has been pointed out elsewhere<sup>36</sup> that using a realistic model for describing the motion of atoms and molecules, rather than using animations based on more or less arbitrary successions of still pictures, carries important advantages from an education viewpoint. The most relevant advantage is that the phenomenon under study is not a preconceived idea but, rather, it is the result of the physical laws ruling the behavior of the system. With this in mind, as explained above, the application was designed as a realistic MD simulation in which simple structureless monoatomic particles move according to Newton’s laws of motion. After a preliminary step, aimed at familiarizing the students with the behavior of a system of non-interacting particles, a realistic interaction potential (see Equation 2) was introduced and attention was mainly focused on the properties of mixtures.

Concepts related to solubility and the processes determining the formation of homogeneous or heterogeneous mixtures are very important in chemistry and, at the same time, they are among the most dif-



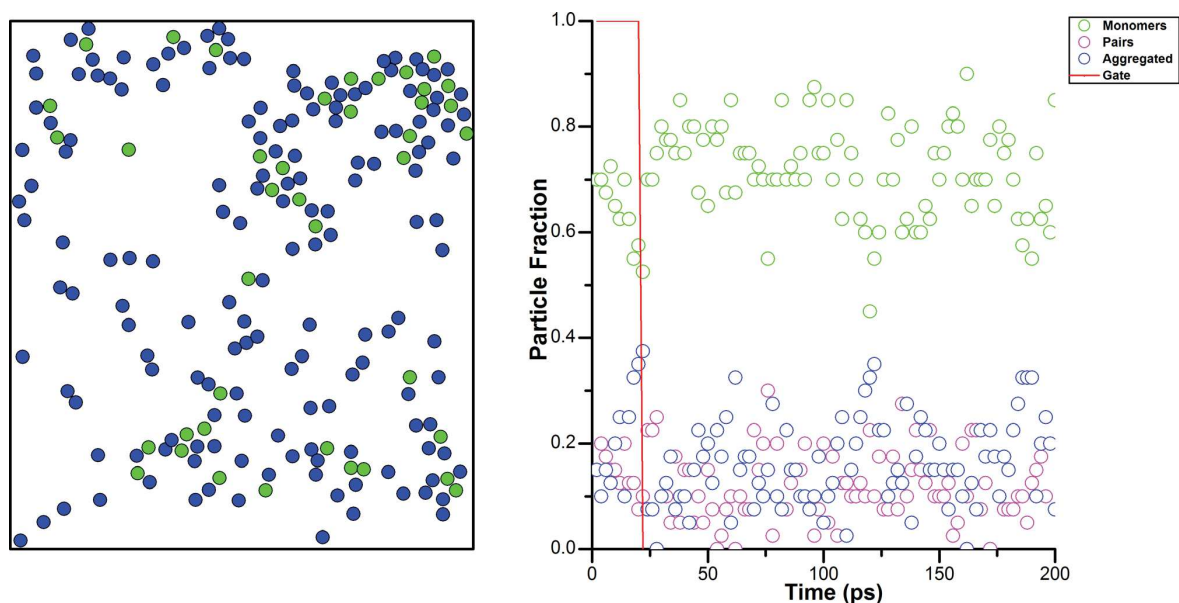
**Figure 5.** Left: snapshots of the configurations obtained after 200 ps (top) and after 400 ps (bottom) of a simulation for the mixture described in Figure 3 at  $T = 300$  K. The interaction parameters (eV) were:  $\epsilon_{A-A} = 0.01$ ,  $\epsilon_{B-B} = 0.1$  and  $\epsilon_{A-B} = 0.05$ . Right: time evolution of the fraction of B monomers, pairs of B atoms and total aggregated B atoms present in clusters of more than 2 B atoms for the same simulation. The time at which the red line sharply drops to zero indicates when the gate shown in Figure 3 was opened and the particles were allowed to mix. The MD time step was 1 fs.

difficult to grasp by the students. A simplified representation, as that adopted in the present work, might be useful because it attributes to different interactions between solute and solvent particles the origin of the dissolution process.

Since the adopted model is based on explicit physical laws, it is possible to change specific parameters and observe the effects of these changes on the phenomenon under investigation. In the case under consideration, i.e. the mixing process of particles of different types, in addition to parameters defining the identity of the particles (size and mass), the relevant variables are tem-

perature and attractive strength parameters. As a consequence, the application was designed to focus on the latter.

Results reported in Figure 4 demonstrate on a qualitative basis, that, when no interactions are present, two different substances will mix at any temperature because there is no reason for particles of one type to favor regions rich of particles of the same type. This idea is a qualitative way of describing the spontaneous process which, from a state consisting of two separate A and B substances, leads to a homogeneous A-B mixture, with a corresponding entropy increase; the instructor will be



**Figure 6.** Left: snapshot of the configuration obtained after 200 ps of a simulation for the mixture described in Figure 3 at  $T = 300$  K. The interaction parameters (eV) were:  $\epsilon_{A-A} = 0.01$ ,  $\epsilon_{B-B} = 0.05$  and  $\epsilon_{A-B} = 0.1$ . Right: time evolution of the fraction of B monomers, pairs of B atoms and total aggregated B atoms present in clusters of more than 2 B atoms for the same simulation. The time at which the red line sharply drops to zero indicates when the gate shown in Figure 3 was opened and the particles were allowed to mix. The MD time step was 1 fs.

able to calibrate the discussion also based on the school level. For high school students, the previous simple explanation will be sufficient, whereas in general chemistry university courses, more detailed references to thermodynamics laws can be made.

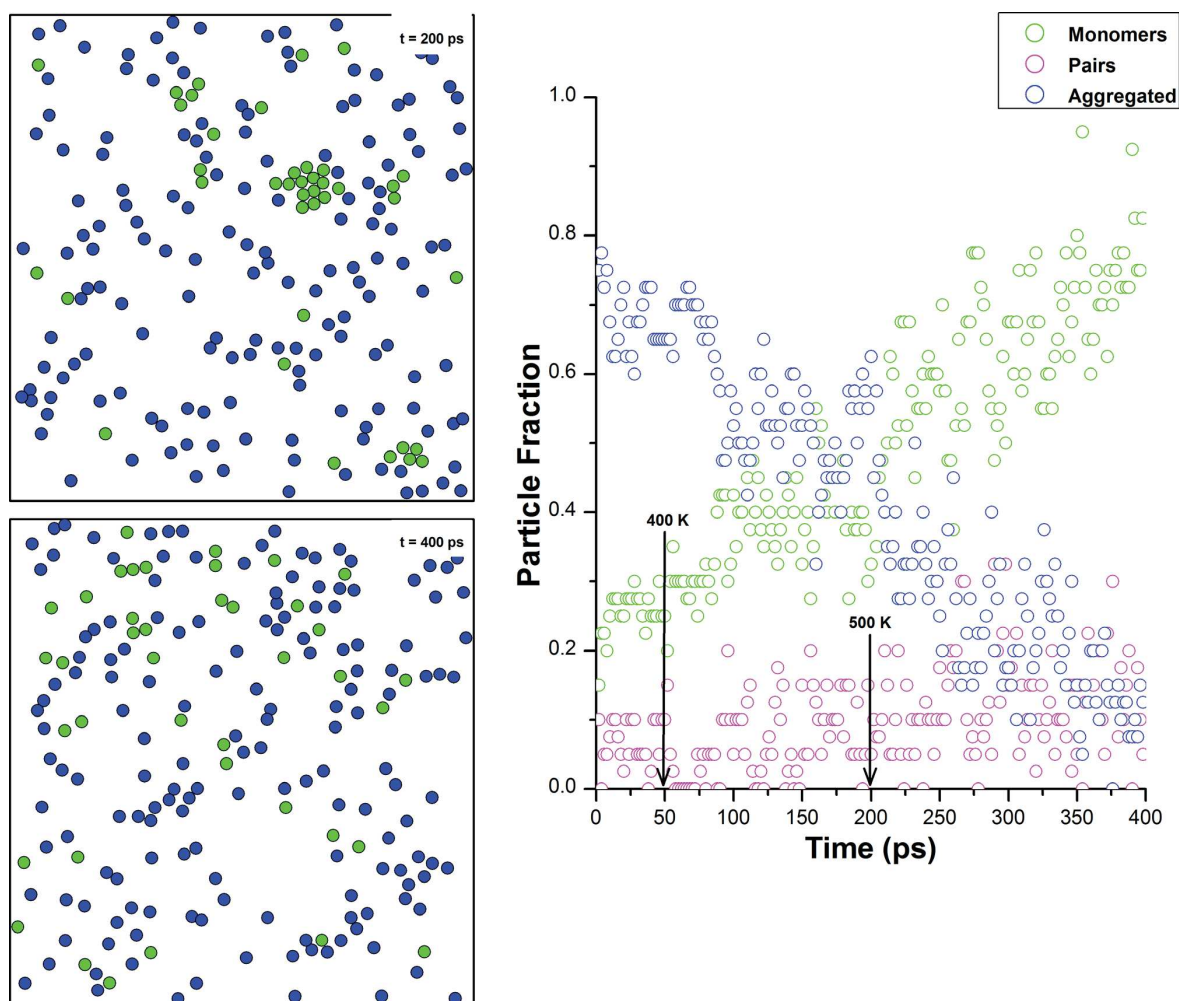
The results reported in Figures 5 and 6 demonstrate the effect of introducing preferential interaction energies between all particle pairs on the resulting mixture. When attractions between solute particles are stronger than those between solute and solvent particles, a heterogeneous mixture will originate in which aggregates of solute particles (a separate phase) are present in a matrix of solvent particles. On the contrary (see Figure 6), when attractions between solute and solvent particles are stronger than those between solute particles, a homogeneous system, i.e. a uniform distribution of solute particles in the matrix of solvent particles, is produced. It is important to underline that, in the two cases just described, the temperature is the same. In other words, the balance between kinetic and potential energies is unchanged. In secondary school chemistry instruction, where very limited thermodynamics concepts are present, the above discussion can be based on considerations similar to those used for explaining transformations of the physical state of a pure substance. Particles (different or alike) attract each other and, as a conse-

quence, they tend to “stick”. At the same time, thermal motion, which is related to the temperature, pushes them apart. Therefore, temperature plays against aggregation and the net result of the competition between these two energy contributions, for a given substance and at a fixed temperature, determines the stable state of the system. Low temperatures favor aggregation and so do large interparticle attractions.

The above discussion is further supported by the results reported in Figure 7, where the temperature was raised and the consequent dissolution of the aggregates, formed at a lower temperature, was obtained. Raising the temperature had the effect of shifting the balance between kinetic and potential energies in favor of the former. The same conclusion can be reached by inspection of the results reported in Figure 8. In this case, the energy balance was in favor of the kinetic term from the beginning of the simulation and, as a consequence, no B-B aggregation was observed.

In summary, in our opinion, the application here presented offers the opportunity of letting the students observe, in an interactive fashion, the basic submicroscopic details underlying a mixing process. It is possible to use the application at different school levels: from the simple qualitative observation of the dynamic configurations, suitable for secondary school classes, to gradually





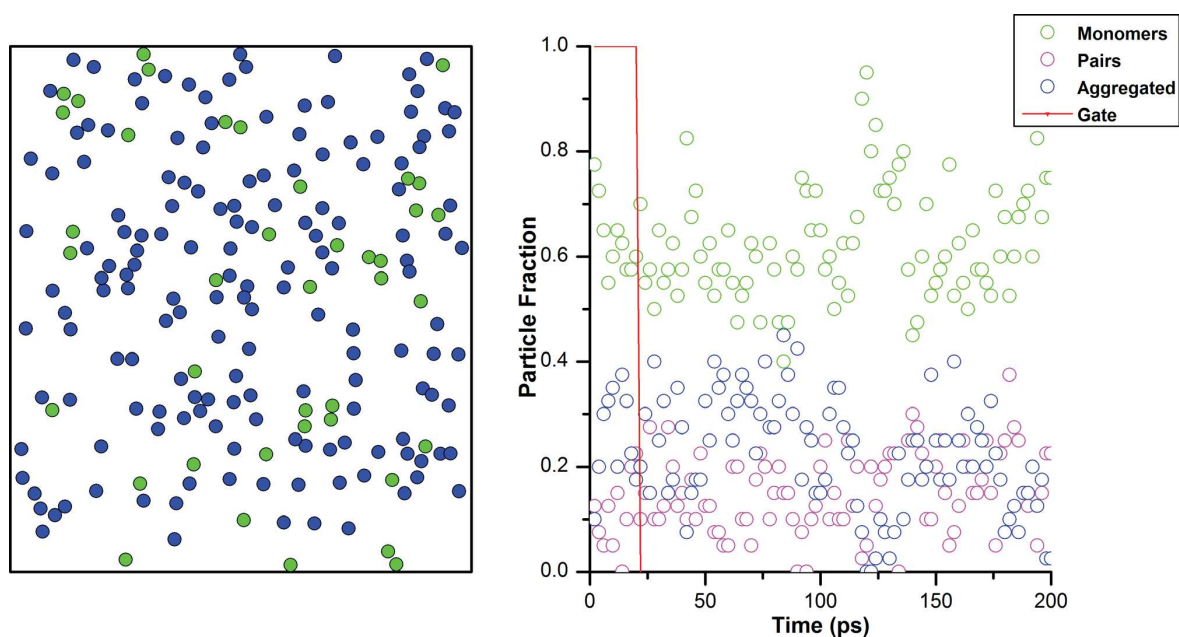
**Figure 7.** Left: snapshots of the configurations obtained after 200 ps (top) and after 400 ps (bottom) of a simulation started from the configuration obtained after 400 ps at the conditions of Figure 5. The mixture was heated at  $T = 400$  K (top) and  $T = 500$  K (bottom). The interaction parameters (eV) were:  $\epsilon_{A-A} = 0.01$ ,  $\epsilon_{B-B} = 0.1$  and  $\epsilon_{A-B} = 0.05$ . Right: time evolution of the fraction of B monomers, pairs of B atoms and total aggregated B atoms present in clusters of more than 2 B atoms for the same simulation. The two arrows indicate the times when the temperature of the simulation was set to the specified values. The MD time step was 1 fs.

more detailed semi-quantitative analysis, also making use of the time evolution of the fractions of the different aggregated species present in the mixture, more appropriate for college general chemistry courses.

In any case, students should be made aware that the observed dynamics are the result of a physically sound model. Actually, in most cases, dynamic illustrations of the sub-macroscopic world generated by animations might be indistinguishable from those produced by a realistic simulation. However, students should be made aware of the difference.

Furthermore, the Java based MD engine<sup>37</sup> here adopted makes it possible to modify and adapt the existing code to special situations and, as a consequence, it is possible to let students' design computer experiments in introductory computational chemistry courses.

Needless to say, the physical description, despite its realistic nature, is very simplified. We propose that adopting a 2D representation does not introduce serious limitations as far as the physical reliability of the model is concerned. However, the very simplified nature of the interaction potential and, for example, the absence



**Figure 8.** Left: snapshot of the configuration obtained after 200 ps of a simulation started from the configuration shown in Figure 3 at  $T = 500$  K. The interaction parameters (eV) were:  $\epsilon_{A-A} = 0.01$ ,  $\epsilon_{B-B} = 0.1$  and  $\epsilon_{A-B} = 0.05$ . Right: time evolution of the fraction of B monomers, pairs of B atoms and total aggregated B atoms present in clusters of more than 2 B atoms for the same simulation. The time at which the red line sharply drops to zero indicates when the gate shown in Figure 3 was opened and the particles were allowed to mix. The MD time step was 1 fs.

of specific interactions among solvent particles, is not suitable for representing special circumstances, such as aqueous solutions, where changes in solvent structure due to the presence of the solute are crucial. It might be recalled, for example, that these structural rearrangements might also lead to a temperature effect on solubility opposite to that predicted by the present model. Nevertheless, such complications might be considered as second order effects with respect to the basic ideas here developed.

#### CONCLUSION

The particle model of matter is a powerful tool for describing the structure and the dynamic properties of matter at the submicroscopic level. With the present application, in our opinion, it is possible to demonstrate in a quite effective way that the study of the dynamic behavior is very often crucial in the understanding of fundamental concepts in chemistry. The adoption of a realistic model, based on classical Newton's laws of motion, rather than using arbitrary animations, offers the added advantage of producing a physically meaningful picture as the outcome of the application of these

laws rather than as a known *a priori* result. As a consequence, system parameters can be freely varied and the effects of these changes on the outcome of the simulation can be systematically investigated.

Depending on the students' background and degree of interest, the instructor will be able to calibrate observations and the subsequent discussion as needed. Even if students are not fully familiar with classical Newton's laws of motion, appropriate qualitative analogies based on common life situations, such as the motion of macroscopic bodies, could be used to clarify these concepts. In more advanced instruction levels, such as introductory general chemistry university courses, students are certainly acquainted with the physics concepts and basic math tools needed for making full use of the application.

Finally, it is worth mentioning that the present model and application is particularly suitable for the study of physical transformation of matter. The structureless nature of the particles rules out the possibility of changes in their chemical identity. Chemical transformations require more refined models.

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