JOURNAL OF CHEMICAL EDUCATION

pubs.acs.org/jchemeduc Article

Elucidating the Influence of the Activation Energy on Reaction Rates by Simulations Based on a Simple Particle Model

Antonella Di Vincenzo and Michele A. Floriano*

Cite This: https://dx.doi.org/10.1021/acs.jchemed.0c00463 Read Online

ACCESS | Metrics & More | Article Recommendations

ABSTRACT: An application for visualizing the dynamic properties of an equimolar binary mixture of isotropic reactive particles is presented. By introducing a user selectable choice for the activation energy, the application is useful to demonstrate qualitatively that the reaction rate depends on the above choice and on temperature. The application is based on a 2D realistic dynamic model where atoms move because of their thermal energies and the trajectories are determined by solving numerically Newton's laws according to a Molecular Dynamics (MD) scheme. Collisions are monitored as time progresses, and every time the collision energy is larger than the selected activation energy, a reactive event occurs. By examining the time evolution of the configurations, it is possible to observe that the number of reactive collisions is always smaller than the total number of collisions. However, the number of reactive events increases on raising the temperature and/or by decreasing the activation energy. The above observations, as well as more quantitative analyses of the simulation data, are useful in elucidating the connections existing among particle kinetic energy, temperature, and activation energy of the reaction. The application can be used at different levels of detail and in different instruction levels. Qualitative visual observations of the progress of the reaction are suitable at all levels of instruction. Systematic investigations on the effect of changes of temperature and activation energy, suitable for senior high school and college courses and useful to gain insight into kinetic models and Arrhenius' law, are also reported.

KEYWORDS: *High School/Introductory Chemistry, First-Year Undergraduate/General, Physical Chemistry, Chemoinformatics, Computer-Based Learning, Kinetics, Kinetic-Molecular Theory*

■ INTRODUCTION

It is well known that, in spite of their relevance in any chemistry curriculum, concepts related to reaction rates and, more generally, to chemical kinetics are among the most difficult to grasp by students at all levels of instruction. Many extensive studies on the presence of alternative conceptions and/or misconceptions have been reported in the past.[1−7] In particular, how the activation energy affects reaction rates appears to be invariably obscure for students and subject to misconceptions.[4,5]

Indeed, many fundamental aspects of chemical kinetics, particularly in gas phase reactions, can be easily and effectively dealt with by applying ideas inspired by the particle model of matter and collision theory.[8−13] For example, for gas phase reactions, while it is probably reasonable for students to accept the idea that reactant molecules must come into contact (i.e., collide) and be properly oriented in order to react, it is not as straightforward to imagine that not all such collisions lead to reaction.

It is relatively simple to demonstrate that, if molecules reacted each time they collide, since the average molecular collision frequency is extremely large ($\approx 10^{30}$ s^{-1}),[14] any chemical transformation should be virtually instantaneous; clearly, this is not the case. In order to calculate the collision frequency, it is necessary to apply the laws of collision theory.[14] However, this number can be roughly estimated by simple considerations. Even young students, at any introductory level chemistry course, should be aware of the fact that a gas is made of atoms/molecules freely moving at a speed, proportional to temperature, of $\sim 10^2-10^3$ m s^{-1}(on an intuitive basis, this number can be compared to the speed of sound in air and, thus, recall how a supersonic bang is produced[15]). It is a useful exercise for students to estimate the order of magnitude of the above collision frequency. A typical gas density ($\approx$1 kg m^{-3}) corresponds to $\approx 10^{25}$ particles m^{-3}, and this implies that the mean distance between particles is $\approx 10^{-8}$ m. As a consequence, each particle (moving at $\approx 10^2$ m s^{-1}) will undergo $\approx 10^{10}$ collisions s^{-1}. Following these ideas, the previous estimate of the overall number of collisions in unit time can be obtained. Once again, if all collisions led to a reactive event, reaction rate should be $\approx 10^6$ mol s^{-1}. On the contrary, typical gas phase reaction rates[16] can vary in a wide range, and they can be as slow as $10^{-4}-10^{-6}$ mol s^{-1}.

Even just on a qualitative and intuitive level, when confronted with the huge difference between the collision frequency and typical gas phase rate constants, students should

Received: May 12, 2020

be able to accept the idea that only a fraction of molecular collisions will produce reactive events.

Further progress in a discussion addressing the reason why collisions may or may not lead to reaction can only be made by introducing molecular energy distributions and activation energy. According to previous studies,[1−7] this is the point where most misconceptions originate and where concepts remain obscure for students.

We propose that students' understanding of the previous concepts can be improved by maintaining a molecular viewpoint combined with macroscopic observations.

In this work, we present a graphical application[17] that combines visual observations of the dynamical behavior of atoms/molecules and semiquantitative estimates of rate constants at different temperatures and/or activation energies. The application can be used to elucidate the energetics involved in chemical kinetics. As we have already pointed out,[18,19] previous studies have used simplified animations where the dynamics were chosen arbitrarily. Here, we expand upon this by introducing a Molecular Dynamics (MD) approach that allows for tuning of the parameters that contribute to reaction rates.

The application can be effectively used at any instruction level where chemical kinetics is part of the curriculum. A simple visual and qualitative approach is suitable for junior high school students whereas, as it will be shown, a more quantitative discussion is aimed at senior high school courses and college chemistry instruction.

■ BASIC PRINCIPLES OF CHEMICAL KINETICS

In this section, the main concepts and laws of chemical kinetics are summarized with particular reference to the specific reaction type that is considered in the present work. More extensive details and general concepts about this topic can be found in the specialized literature.[16,20,21]

The reaction type here considered can be written as

$$\mathrm{A} + \mathrm{B} \rightarrow \mathrm{C} \tag{1}$$

where A, B, and C can be atomic and/or molecular species.

For this particular case, the reaction rate, r, can be defined as

$$r = -\frac{\mathrm{d[A]}}{\mathrm{d}t} = -\frac{\mathrm{d[B]}}{\mathrm{d}t} = \frac{\mathrm{d[C]}}{\mathrm{d}t} \tag{2}$$

where [A], [B], and [C] are the concentrations of each species.

The dependence of the reaction rate on the concentrations of the reacting species is expressed by the rate law of the reaction. It is important to underline that, in general, this law can only be determined experimentally since the stoichiometric equation only describes the overall process which might be the result of a variable number of intermediate steps. However, if we assume that reaction 1 results from the direct encounter of A and B molecules to produce the product C, i.e., we are dealing with a *bimolecular* process, the reaction rate is proportional to A and B concentrations; as a consequence, the kinetic law can be written as

$$r = k[\mathrm{A}][\mathrm{B}] \tag{3}$$

where k is a temperature dependent rate constant. In this case, the reaction is first order in A and first order in B.

In general, depending on the reaction mechanism, the effect of temperature on the rate constant k can only be assessed from experimental observations which also suggest possible reaction mechanisms. For many reactions, the temperature dependence of the rate constant k is described by Arrhenius' law:

$$k = Z \exp\left(-\frac{E_a}{RT}\right) \tag{4}$$

where R is the ideal gas constant, T is the absolute temperature and, at least in its original empirical formulation, Z and E_a, known as pre-exponential factor and activation energy, respectively, are reaction specific empirical parameters which, as we will discuss later, may assume a physical interpretation depending on the model used. Arrhenius' law certainly holds for the special case of the *bimolecular* process under consideration here.

According to eq 4, a plot of ln k vs $1/T$ is a straight line with intercept equal to ln Z and slope equal to $-E_a/R$. Arrhenius' law predicts that the reaction rate increases with an increase in the temperature.

In the simple case of gas phase reactions, the collision theory[8−12,20,22] provides an interpretation of Arrhenius' law by identifying the parameter Z as a slightly temperature dependent collision frequency and E_a as the minimum collision energy required for a reactive encounter.

In summary, the key point that must be clarified essentially deals with the fact that the molecular kinetic energy is connected to thermal motion (the average molecular speed increases with temperature and decreases with molecular mass). Molecular energies are distributed according to the Maxwell−Boltzmann equation:[20,23]

$$f(E) = 2\sqrt{\frac{E}{\pi}}\left(\frac{1}{RT}\right)^{3/2} \exp\left(-\frac{E_a}{RT}\right) \tag{5}$$

where $f(E)$ is the fraction of molecules with kinetic energy in the range E and $E + \mathrm{d}E$, R is the ideal gas constant, and T is the absolute temperature. A reactive event generally implies breaking chemical bonds in the reactant molecules, and this process requires energy. As a consequence, only collisions involving sufficient energy can produce a reaction. Within this simple collision model, the activation energy is introduced as the minimum collision energy required in order to obtain the products.

In Figure 1, the energy distributions at three different temperatures are reported, and they are compared with an arbitrary activation energy value.

Plots of this kind are often used[22,24,25] to demonstrate that only a fraction of the total number of reactant molecules are energetic enough to react. However, since what is significant is whether a given binary collision would be sufficiently energetic, rather than the consideration of the single molecule energy distribution, it would be more appropriate to take into account a collision energy distribution. Deriving such a distribution function is a rather complicated task[23] whose final result is

$$f(\varepsilon) = \exp\left(-\frac{\varepsilon_0}{kT}\right) \tag{6}$$

where $f(\varepsilon)$ is the fraction of the collisions of energy $\varepsilon \geq \varepsilon_0$, an arbitrary threshold energy value equivalent to the activation energy.

For reactions in condensed phases, the above discussion, on the basis of occasional binary collisions of otherwise freely moving molecules, does not apply. In these cases, transition state theory is used, and the Arrhenius activation energy is associated with the energy of an activated complex.[16,21,22,25,26]

https://dx.doi.org/10.1021/acs.jchemed.0c00463
J. Chem. Educ. XXXX, XXX, XXX−XXX

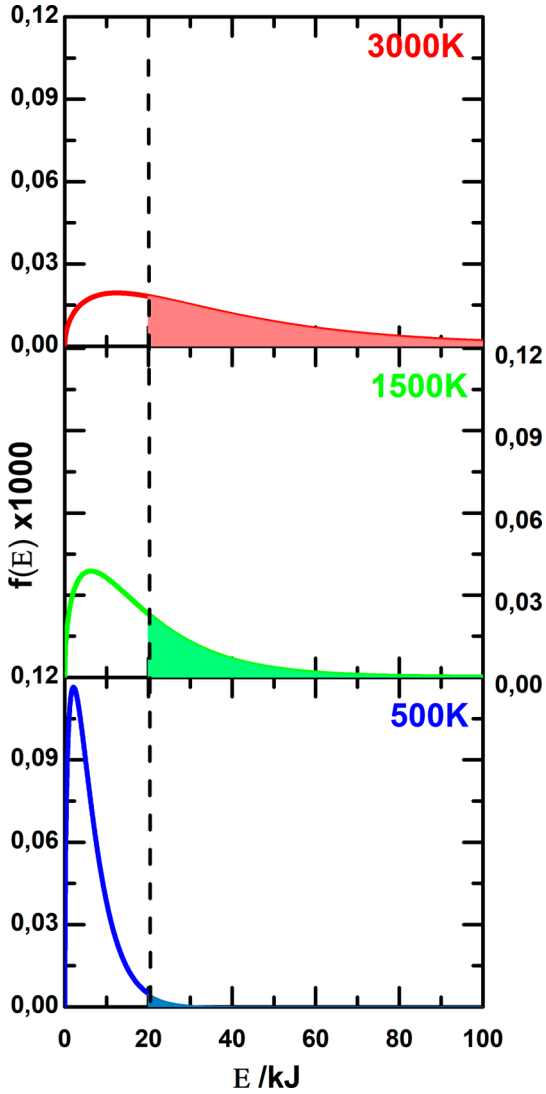

Figure 1. Fractions of molecules with kinetic energy in the range E and $E + dE$, $f(E)$, as functions of molecular kinetic energy E at the indicated temperatures. Colored areas indicate the fractions of molecules with $E \geq 20$ kJ mol^{-1} (dashed line).

Reactions in condensed phases are not of interest in the present work, and they will not be considered further.

As has been pointed out already,[1−7] the above discussion is the origin of important misconceptions which prevent students from gaining a thorough, even if only qualitative, understanding of the subject. In particular, among all other possible misconceptions in chemical kinetics, a relevant number of students seems to think that the activation energy is the kinetic energy of the reagents or that it represents the energy released in a chemical transformation. In addition, many students miss the connections among temperature, activation energy, and reaction rate.

The application presented[17] in this work has been designed to address and, hopefully, prevent some of the above conceptual hurdles.

■ SUMMARY OF COMPUTATION DETAILS

For the reasons discussed in previous work,[18,19] in order to describe and visualize the dynamical behavior of the particle model of matter, rather than use arbitrary animations, in this work a realistic model based on the Molecular Dynamics (MD) method has been adopted. In this way, in addition to the didactical advantage of demonstrating how a theoretical model can provide quantitative tools by the use of explicit physical laws, control parameters can be changed systematically in order to investigate the effects on the results.

In the application presented here,[17] the same number of structureless noninteracting particles of types A and B of diameter $\sigma_A = 1.4$ Å and $\sigma_B = 2.1$ Å and mass $m_A = 40$ g mol^{-1} and $m_B = 60$ g mol^{-1} moves in a bidimensional simulation cell 60×60 Å^2 with an associated kinetic energy proportional to the absolute temperature T (K). In an MD simulation, the position and velocity of each atom can be calculated, for a given time step $dt = 1$ fs, by solving numerically Newton's equations of motion. Full details about the MD procedure can be found in previous work[18,19] and in the specialized literature.[27,28] In this work, a web-based MD engine[29] was used.

In summary, in the simple case here under study, namely, a mixture of the same number of A and B structureless particles, all the user has to do in order to start the simulation is select one of the three available numbers n of particles to be considered in the simulation, set the temperature T to the desired value within the specified range, and, finally, choose one of the available options for the activation energy E_a indexed from 1 to 4 in order of increasing E_a. The initial positions of the n particles are randomly chosen.

In principle, an MD simulation can be performed in two or three dimensions, with the latter being more realistic but computationally substantially more demanding.[18] In this work, in order to minimize the computing time and, thus, run the application interactively, a 2D environment was adopted.

An accurate and detailed treatment of the reaction dynamics laws is well beyond the scope of the present work, and full details can be found in the specialized literature.[30−32] In the simple description of the influence of the activation energy on the reaction rate summarized in the previous section, in the present application no chemical bonds are explicitly broken or formed. According to reaction 1, collisions between A and B particles are monitored at fixed time intervals (100 fs). Every time an A and a B particle are at the contact distance, the sum of their respective kinetic energies $E_A + E_B$ is compared with the preselected value of the activation energy E_a. If $E_A + E_B > E_a$, the two colliding particles are replaced by a new particle C with $\sigma_C = 2.1$ Å and mass $m_C = 100$ g mol^{-1}. The two colliding particles are considered to be within reaction distance when

$$r_{AB} < \gamma \frac{\sigma_A + \sigma_B}{2} \tag{7}$$

where r_{AB} is the hard-sphere distance between the A and B centers of mass and γ is a dimensionless parameter introduced in order to allow for softer collisions. In this work, $\gamma = 1.1$.

Obviously, in this simplified picture, no effects such as the orientation of the collision or the directions of the colliding particles are taken into account and, as a consequence, the number of reactive events is probably overestimated.

When the application starts, it is possible to observe in the simulation box that the two different kinds of particles move for a duration of 50 ps without producing any reaction. This is done in order to equilibrate the system and to ensure that an equilibrium Maxwell−Boltzmann distribution at the specified temperature is attained. After this preliminary stage, product particles begin to be formed. The two plots on the right-hand

https://dx.doi.org/10.1021/acs.jchemed.0c00463
J. Chem. Educ. XXXX, XXX, XXX−XXX

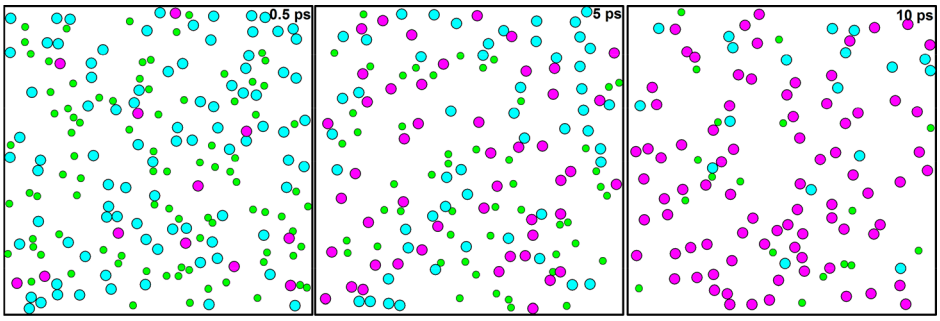

Figure 2. Sample configurations of a simulation started with 100 A (green) and 100 B (blue) particles and producing C (pink) particles according to eq 1 after the indicated times (ps). A and B particles were allowed to react after a 50 ps equilibration stage (see text). Particle parameters were as follows: σ (Å) = 1.4, 2.1, 2.1, and m (g mol^{-1}) = 40, 60, 100, for A, B, and C, respectively. Initial A and B positions were randomly selected.

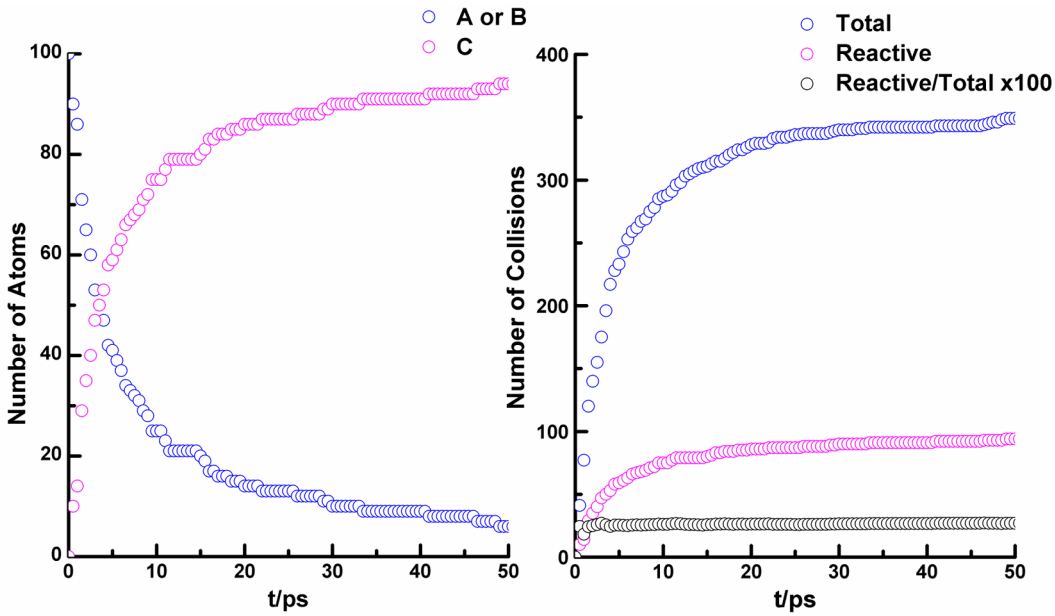

Figure 3. Left: Time evolution of the number of B (the same as the number of A) and of C particles. Right: Time evolution of the number of total and reactive collisions (see text) and of the ratio between these two quantities. All data refer to the same simulation of Figure 2.

side of the computer screen show the time evolution of the number of reactant and product particles and that of the number of collisions. In our opinion, this simultaneous evidence of the particle dynamics and the corresponding change in time of the number of reacting species enhances the connection between the particles' behavior and its overall description.

■ RESULTS AND DISCUSSION

As pointed out in the Introduction, the present application can be used at different detail levels, and thus, it can be adapted to different instruction levels. An introductory qualitative approach simply consists of observing the rate of formation of C (pink) particles at the expense of A (green) and B (blue) particles at given T and E_a values. Once the application starts, after the equilibration stage described above during which A and B particles are simply moving and colliding with each other and with the simulation cell boundaries, product C begins to form. Students should be encouraged to observe that not all A and B collisions lead to the formation of C particles. In Figure 2, sample configurations for a simulation performed at the specified conditions are shown.

The two plots on the right (see Figure 3) are useful in order to integrate the above qualitative observations with a more quantitative approach.

In the first plot, the time evolutions of the number of B and C particles are displayed. In the second plot, the time evolutions of the number of total A and B collisions, of the number of A and B collisions energetic enough to lead to the formation of the product C, and of the ratio between these two quantities are shown. The fact that the ratio between the number of reactive collisions ($E_A + E_B > E_a$) and the number of total collisions is <1 supports the previous discussion.

The above observations can be repeated at different temperatures at a fixed E_a value and, alternatively, using the different E_a available options at a fixed temperature. Incidentally, the actual E_a values (kJ mol^{-1}), 10, 20, 40, and 80, corresponding to the different possible selections from E_{a1} to E_{a4}, are not known by the user. As will be discussed later, these values will be calculated from numerical data obtained by a systematic use of the application. It should be possible to observe that the rate of formation of C particles increases, i.e., they are formed more rapidly, on increasing the temperature or by decreasing the activation energy. The rate of formation of C

https://dx.doi.org/10.1021/acs.jchemed.0c00463
J. Chem. Educ. XXXX, XXX, XXX−XXX

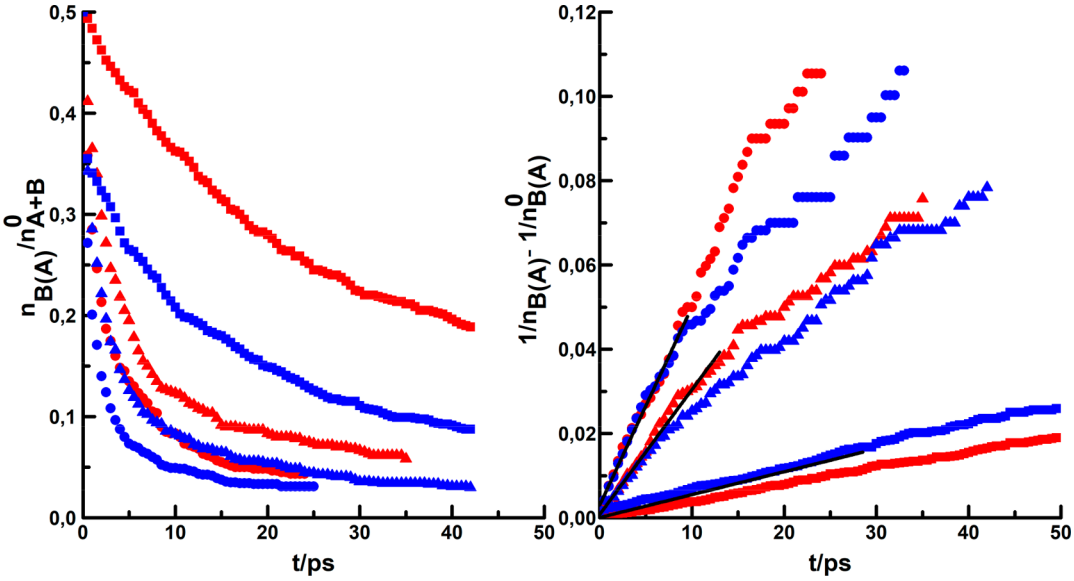

Figure 4. Left: Time evolution of the number of B (the same as the number of A) particles, n_B, with respect to the total initial number of A and B particles, n^0_{A+B}. Right: Second order kinetic law plots (see text). Data were obtained with n^0_{A+B} = 200 (red symbols) and n^0_{A+B} = 400 (blue symbols), and different E_a options are as follows: E_{a1}(circles), E_{a2} (triangles), and E_{a3} (squares). The temperature was T = 1000 K, and the particle parameters were the same as those of Figure 2. Black lines represent linear fits to the experimental points according to eq 9. The obtained rate constant k (10^9 n^{-1} s^{-1}) values were 4.71 (0.09), 2.96 (0.05), and 0.54 (0.02) in order of increasing E_a. In parentheses, uncertainties are also reported.

particles can be estimated by a visual inspection of the configurations such as those shown in Figure 2 and/or by analyzing the amount of product present after the same time following the beginning of the reaction at the different adopted conditions. It might be pointed out that, as indicated by reaction 1, for each C particle formed, one A and one B particle are lost. As a consequence, as indicated by eq 2, the rate of formation of the product C is the same as the rate of consumption of A or that of B. It should be pointed out that an increase in the reaction rate corresponds to a larger fraction of reactive collisions with respect to the total number, and this can be achieved either by increasing the temperature, corresponding to an increase of the average kinetic energy of the particles, and/or by decreasing the activation energy E_a.

Further data analysis, suitable for upper high school and introductory college chemistry courses, provides additional insight about the kinetic laws and the connections among reaction rate, temperature, and activation energy. The numerical data required for the following discussion can be obtained as spreadsheet columns, by following the instructions given in the application.

Because of the small number of particles involved, results from the application might be affected by relatively large uncertainties. For this reason, results presented here are always averages of at least three independent simulations.

In general, the rate constant can be derived by integration of eq 3. In the case under consideration, namely, an equimolar mixture of A and B particles, the rate law can be written as

$$r = -\frac{dn_A}{dt} = -\frac{dn_B}{dt} = kn_A^2 = kn_B^2 \tag{8}$$

The integrated form of this kinetic law is

$$\frac{1}{n_A} - \frac{1}{n_A^0} = \frac{1}{n_B} - \frac{1}{n_B^0} = kt \tag{9}$$

In Figure 4, in the plot on the left, the effect of increasing E_a at a fixed T is illustrated. Since different initial numbers of A and B particles were used, data are reported as fractions with respect to the initial total number of particles, n^0_{A+B}. The time evolutions of the fractions of the number of B particles (the same as the number of A particles) with respect to the initial total number of particles are reported for the different specified conditions. First of all, by comparing the fractions of unreacted B particles at the same simulation time and/or the time needed for complete reaction, immediate qualitative observations suggest that the reaction is faster when the initial number of reactant species is larger and when E_a is smaller. In the plot on the right, the same data are reported in the form indicated by eq 9.

As shown in the figure, from the linear fits of these data, the rate constant, k, values can be obtained.

Appropriate simulations can be performed for each E_a option at different temperatures, in order to produce Arrhenius plots similar to those shown in Figure 5.

The slopes of the linear fits are proportional to the different E_a values. Even though the user is not aware of the actual E_a values (10, 20, 40, and 80 kJ mol^{-1}) used in the different simulation, it is worth mentioning that the calculated values (see legend of Figure 5) are consistently smaller than the actual ones. In other words, the actual rate constants and their temperature dependence correspond to smaller E_a values; i.e., the fraction of collisions energetic enough to produce reactive events is larger than the expected ones. Given the physically unrealistic collision model and its 2D nature adopted here, the drastic approximations introduced, and the small sample sizes, the above differences are not surprising. Since the main purpose of the application presented here is to elucidate, in a semiquantitative way, the energy factors affecting the reaction rate, a rigorous and more accurate description is not necessary. However, obtaining calculated E_a values different from those sets at the start of the simulation might be confusing for the students, and for this reason, the latter are not explicitly stated in the application. Furthermore, this offers to students useful data analysis opportunities.

https://dx.doi.org/10.1021/acs.jchemed.0c00463
J. Chem. Educ. XXXX, XXX, XXX−XXX

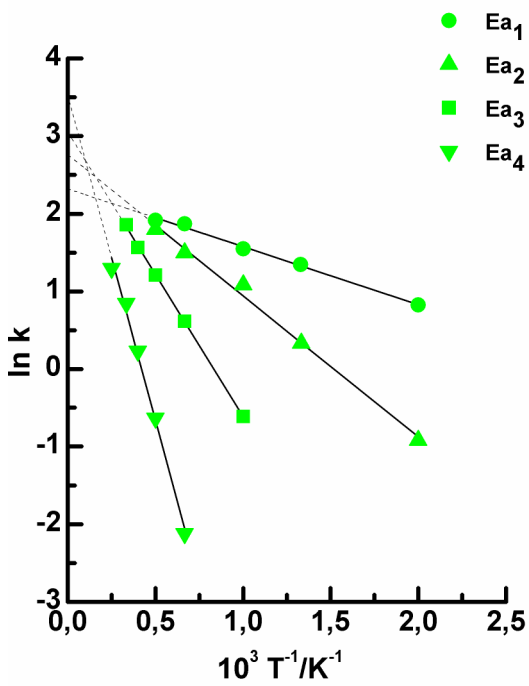

Figure 5. Arrhenius plots (see text) of rate constant, k, values obtained from linear fits similar to those shown in Figure 4 at different T and E_a options specified in the legend. E_a values (kJ mol^{-1}), calculated from the slopes of the linear fits (black solid lines), were 6.2 (0.3), 15.1 (0.7), 30.5 (0.3), and 70 (3). In parentheses, uncertainties are also reported. Dashed black lines are extrapolations of the fits.

At this point of the discussion, it is important to point out an aspect of the influence of E_a on reaction rates. Reactions with large E_a values are more sensitive to changes in T. This is an area which students have difficulty with,[3] since the rate constant for a reaction with a higher E_a will increase by a larger factor than the rate constant for a reaction with a smaller E_a.

The observed increase in the intercepts of the linear fits is, at least in part, attributable to the larger T values needed to obtain reasonable reaction rates at large E_a values. In fact, in the interpretation within the collision theory,[20] the Arrhenius' pre-exponential parameter is identified as a slightly temperature dependent collision frequency.

Further evidence about the fact that the reaction rate increases on increasing the temperature and/or decreasing the activation energy, because of the larger fraction of reactive collisions, is obtained from the data reported in Figure 6. Here, the time evolutions of the fractions of the number of A and B collisions with respect to that observed at the beginning of the reaction (t = 500 fs), f_{coll}, as well as that of the fraction of reactive collisions with respect to the total number, f_r, are reported at different temperatures and a fixed E_a value (left) and at different E_a values at a fixed T (right).

It can be observed that, in all cases, as the reaction evolves, due to the formation of the product C, the number of A and B collisions decreases because of the decreasing number of A and B particles. However, the fraction of reactive collisions remains constant. As expected, the fraction of reactive collisions increases on increasing the temperature and/or on lowering the activation energy.

■ SUMMARY

Because of its relevance in practical applications and its power in elucidating reaction mechanisms, chemical kinetics is a quite important topic in chemical education. However, as discussed in the Introduction, many studies, as well as personal experience, have demonstrated that students have trouble conceptualizing even the simplest kinetic laws and that alternative conceptions of different kinds are present. One of the most common hurdles is realizing that, in spite of the fact that in a simple gas phase reaction a very large number of collisions among the reactant species occurs, the rate of

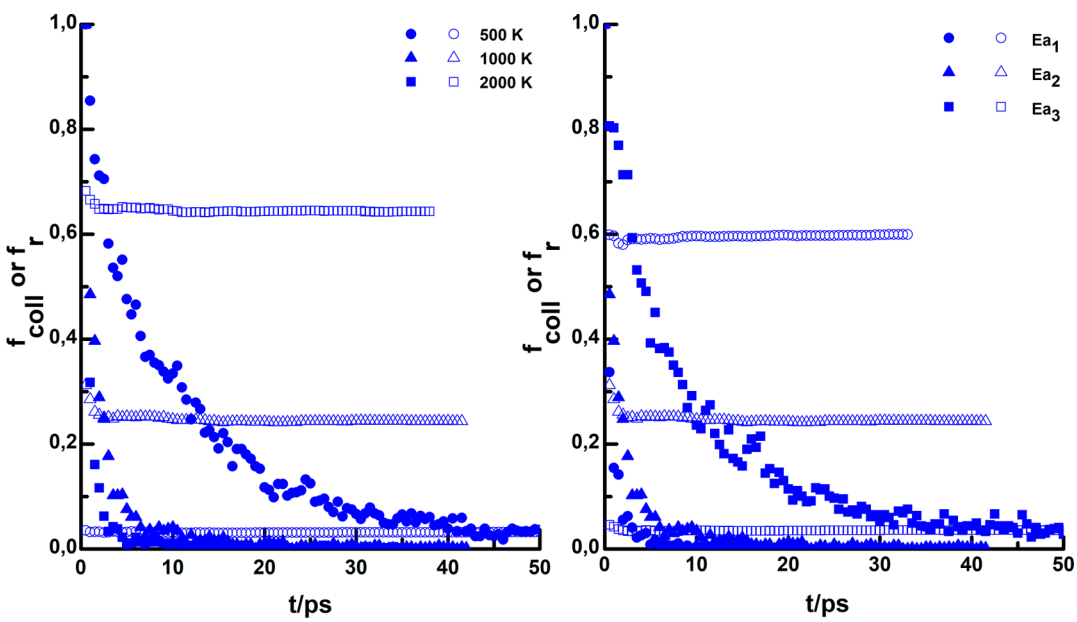

Figure 6. Time evolutions of the fractions of the number of A and B collisions with respect to that at t = 500 fs, f_{coll} (solid symbols), and that of the fraction of reactive collisions with respect to the total number, f_r (open symbols). Left: $E_a = E_{a2}$ and temperatures specified in the legend. Right: T = 1000 K and E_a options specified in the legend.

https://dx.doi.org/10.1021/acs.jchemed.0c00463
J. Chem. Educ. XXXX, XXX, XXX−XXX

formation of the products can be quite small. This is usually explained by stating that the energy required to break bonds in the reactant molecules, a propaedeutic stage in order to form new ones in the product molecules, in the gas phase arises from the kinetic energy of the colliding molecules which, as a consequence, must be large enough. This discussion leads to the introduction of a reaction specific activation energy, a threshold energy that must be overcome by a large enough kinetic energy (i.e., temperature) of the reactant molecules.

In the present work, in an attempt to overcome some of the difficulties encountered by students in addressing properly the above topic and relying on the education power of visualizations based on the particle model of matter, a graphical application has been designed and implemented.

It is assumed that, by visualizing time lapse sequences of molecular trajectories and the subsequent collisions, it is possible to illustrate visually that only a fraction of these collisions results in reactive events. Furthermore, in the present application, rather than using cartoon-like animations based on more or less arbitrary dynamic laws, a realistic MD scheme was adopted.

It is expected that, after becoming familiar with the connection between the number of effective collisions and the chemical rate of a simple gas phase reaction by the use of the application presented here, students will be able to use more efficiently other available kinetics simulators[33,34] dealing with more complex systems. The application uses a web-based MD engine, and thus, it can be used even on commonly available tools such as tablets and smartphones; as a consequence, it is easily accessible to a wide audience.

The application has been designed in order to address the connection existing between the rate of a simple bimolecular gas phase reaction and temperature by introducing a threshold collision energy value necessary in order to obtain a reaction.

At an introductory level of instruction, where kinetic laws are probably not presented in detail, qualitative observations of the number of product molecules formed (or, because of the simple reaction considered, of the number of reactant molecules consumed) in a given time interval allow an estimation of the reaction rate. By changing the temperature and/or the activation energy, it is possible to connect these changes easily with their effects on the reaction rate. For the given conditions, it can be readily observed that A and B particles are in constant collision with each other, but only some of the collisions produce a reactive event. Depending on the T and E_a values selected, the time needed to form a given number of product particles varies, and it will be apparent that high temperatures and small activation energies will make the reaction faster. An additional important observation is that the particles move faster as the temperature is raised. Students should be encouraged to connect faster moving particles with a larger average kinetic energy and, on the average, more energetic collisions. Such visual qualitative observations of the configurations are easily integrated with the two plots simultaneously displayed while the application runs. From these plots, students should be asked to estimate the reaction rate and, as a consequence, suggest ways of defining such a quantity.

Older high school students might be familiar enough with Newton's laws to appreciate the realistic nature of the proposed MD model. In any case, they should be able to perform the simple data manipulation tasks required for more quantitative analyses of the simulation data. In so doing, they should be able to test the basis of Arrhenius' law and, more generally, of temperature activated processes.

Finally, in college level courses, students might be guided in more detailed investigations about the connections among temperature, the Maxwell−Boltzmann energy distribution, and its significance in terms of activation energy. Since the scripts required to control and adapt the general-purpose MD engine adopted here are coded in the Java language, in more advanced computational chemistry courses, it might be possible to modify the application in order to deal with specific tasks.

The present application has been preliminarily tested by a small number of college students in an introductory physical chemistry course and by several high school chemistry teachers and satisfactory feedback comments were obtained. Furthermore, it has been tested by eight master students attending a chemistry education course. The application was introduced after a general discussion about the principles dealing with the effect of the activation energy on reaction rates. Following the use of the present application, a similar discussion demonstrated that students had improved their understanding, and by their own admission, the dynamic visualization of the colliding particles had a major impact on their perception of the reaction mechanism. A systematic investigation of its introduction in junior and senior high school chemistry courses is planned.

■ AUTHOR INFORMATION

Corresponding Author

Michele A. Floriano − *Dipartimento di Scienze e Tecnologie Biologiche, Chimiche e Farmaceutiche, Università degli Studi di Palermo, 90128 Palermo, Italy;* orcid.org/0000-0003-0340-0301; Email: michele.floriano@unipa.it

Author

Antonella Di Vincenzo − *Dipartimento di Scienze e Tecnologie Biologiche, Chimiche e Farmaceutiche, Università degli Studi di Palermo, 90128 Palermo, Italy*

Complete contact information is available at:
https://pubs.acs.org/10.1021/acs.jchemed.0c00463

Notes

The authors declare no competing financial interest.

■ REFERENCES

(1) Justi, R. Teaching and Learning Chemical Kinetics. In *Chemical Education: Towards Research-Based Practice*; Gilbert, J. K., De Jong, O., Justi, R., Treagust, D. F., Van Driel, J. H., Eds.; Springer Netherlands: Dordrecht, 2003; pp 293−315.

(2) Cakmakci, G. Identifying Alternative Conceptions of Chemical Kinetics among Secondary School and Undergraduate Students in Turkey. *J. Chem. Educ.* **2010**, *87* (4), 449−455.

(3) Bain, K.; Towns, M. H. A review of research on the teaching and learning of chemical kinetics. *Chem. Educ. Res. Pract.* **2016**, *17* (2), 246−262.

(4) Yan, Y. K.; Subramaniam, R. Diagnostic appraisal of grade 12 students' understanding of reaction kinetics. *Chem. Educ. Res. Pract.* **2016**, *17* (4), 1114−1126.

(5) Yan, Y. K.; Subramaniam, R. Using a multi-tier diagnostic test to explore the nature of students' alternative conceptions on reaction kinetics. *Chem. Educ. Res. Pract.* **2018**, *19* (1), 213−226.

(6) Gegios, T.; Salta, K.; Koinis, S. Investigating high-school chemical kinetics: the Greek chemistry textbook and students' difficulties. *Chem. Educ. Res. Pract.* **2017**, *18* (1), 151−168.

(7) Lamichhane, R.; Reck, C.; Maltese, A. V. Undergraduate chemistry students' misconceptions about reaction coordinate diagrams. *Chem. Educ. Res. Pract.* **2018**, *19* (3), 834−845.
(8) Evenson, A. Putting Reaction Rates and Collision Theory in the Hands of Your Students. *J. Chem. Educ.* **2002**, *79* (7), 822.
(9) McAlduff, E. J. An introduction to collision theory rate constants via distribution functions. *J. Chem. Educ.* **1980**, *57* (9), 627.
(10) Reid, K. L.; Wheatley, R. J.; Horton, J. C.; Brydges, S. W. Using Computer Assisted Learning to Teach Molecular Reaction Dynamics. *J. Chem. Educ.* **2000**, *77* (3), 407.
(11) Smith, I. W. M. A new collision theory for bimolecular reactions. *J. Chem. Educ.* **1982**, *59* (1), 9.
(12) Sweeder, R. D.; Herrington, D. G.; VandenPlas, J. R. Supporting students' conceptual understanding of kinetics using screencasts and simulations outside of the classroom. *Chem. Educ. Res. Pract.* **2019**, *20* (4), 685−698.
(13) Iribe, J.; Hamada, T.; Kim, H.; Voegtle, M.; Bauer, C. A. Rolling the Dice: Modeling First- and Second-Order Reactions via Collision Theory Simulations in an Undergraduate Laboratory. *J. Chem. Educ.* **2020**, *97*, 764.
(14) Laurendeau, N. M. Kinetics of Molecular Transport. In *Statistical Thermodynamics: Fundamentals and Applications*; Cambridge University Press, 2010.
(15) Lilley, G. M.; Westley, R.; Yates, A. H.; Busing, J. R. The Supersonic Bang. *Nature* **1953**, *171* (4362), 994−996.
(16) Atkins, P.; de Paula, J. The rates of chemical reactions. In *Physical Chemistry*, 9th ed.; Oxford University Press: Great Britain, 2010; p 782.
(17) Reaction Rate and Activation Energy. http://www1.unipa.it/flor/MW/Activation_install.pdf (accessed 27/02/2020).
(18) Di Vincenzo, A.; Floriano, M. A. Realistic Implementation of the Particle Model for the Visualization of Nanoparticle Precipitation and Growth. *J. Chem. Educ.* **2019**, *96*, 1654.
(19) Antonella Di, V.; Michele, F. Realistic Visualization of Solubility by the Particle Model for Chemistry Education. *Substantia* **2019**, *3* (2). DOI: 10.13128/Substantia-511
(20) Atkins, P.; de Paula, J. Reaction dynamics. In *Physical Chemistry*, 9th ed.; Oxford University Press: Great Britain, 2010; p 831.
(21) Hammes, G. G. *Principles of Chemical Kinetics*; Elsevier Academic Press, 1978.
(22) House, J. E. Reactions in the Gas Phase. In *Principles of Chemical Kinetics*, 2nd ed.; Press, A., Ed.; Elsevier Academic Press: Burlington, MA, 2007; pp 111−152.
(23) Laurendeau, N. M. *Statistical Thermodynamics: Fundamentals and Applications*; Cambridge University Press, 2010.
(24) Atkins, P.; Paula, J. D. Chemical kinetics: the rates of reactions. In *Elements of Physical Chemistry*, 5th revised ed.; Oxford University Press: Oxford, United Kingdom, 2009; pp 219−243.
(25) Benson, C. Chemical Kinetics. In *Physical Chemistry*, 1st ed.; Global Media: Bhagirath Palace, Chandni Chowk, Delhi, 2009; pp 19−89.
(26) Upadhyay, S. K. Reaction Dynamics. In *Chemical Kinetics and Reaction Dynamics*; Springer: Dordrecht, 2006; pp 204−245.
(27) Allen, M. P.; Tildesley, D. J. *Computer Simulations of Liquids*; Clarendon Press: New York, 1987.
(28) Leach, A. R. *Molecular Modeling: Principles and Applications*, 2nd ed.; Pearson Education, 2001.
(29) Xie, C. Visual, Interactive Simulations for Teaching & Learning Science. http://mw.concord.org/modeler/ (accessed Febrary 2019).
(30) Levine, R. D. *Molecular Reaction Dynamics*; Cambridge University Press: Cambridge, 2005.
(31) Niels, E. H.; Hansen, F. Y. *Theories of Molecular Reaction Dynamics: The Microscopic Foundation of Chemical Kinetics*, 2nd ed.; Oxford University Press, 2018.
(32) Xie, Q.; Tinker, R. Molecular Dynamics Simulations of Chemical Reactions for Use in Education. *J. Chem. Educ.* **2006**, *83* (1), 77.
(33) Peng, Z.; Jimenez, J. KinSim: A Research-Grade, User-Friendly, Visual Kinetics Simulator for Chemical-Kinetics and Environmental-Chemistry. *J. Chem. Educ.* **2019**, *96* (4), 806−811.
(34) da Silva Júnior, J.; Sousa Lima, M. A.; Sousa, E.; Oliveira Alexandre, F.; Leite Júnior, A. KinChem: A Computational Resource for Teaching and Learning Chemical Kinetics. *J. Chem. Educ.* **2014**, *91* (12), 2203−2205.

https://dx.doi.org/10.1021/acs.jchemed.0c00463
J. Chem. Educ. XXXX, XXX, XXX−XXX