

Learning goals for Reactions and Rates simulation: The numbered items are measurable learning goals that the development team wrote. Some hints for the teacher are provided under the bullets items.

First panel, Single Collision

**1. Describe reactions in terms of a simple molecular model.**

- For this goal, I want the students to use the model presented on the **Simple Collision** tab. This is not a model that is presented in texts, but the PhET team thought that a 1D model might help students focus on just a few things: not all collisions result in a new substance and reactions are reversible. Reactions are the result of collisions and the products may collide and react to give reactants

**2. Explain how the simulation model relates to test tube size experiments**

- Real reaction vessels don't have a molecular shooter, what is it modeling? Explain how you used it to test your ideas about how reactions occur.
- When you pull out the shooter, it acts like stretching a spring so the molecule gets elastic potential energy; when you let go, the energy is converted to Kinetic energy and gives the molecule speed just like heating the container would.
- The shooter could represent pouring the substances together and stirring with variable vigor.

**3. Students will describe on a microscopic level, what contributes to a successful reaction. (Include illustrations)**

- Make sure your students pull the shooter a variety of distances and change the angle
- Reactions are the result of collisions between molecules. Whether a collision leads to products or not is determined by both the speed (energy) and angle of the collision. It may be difficult for the students to see the effect of the angle, but if you have the shooter on an angle and pull it out so that the Total energy is above the activation energy, the collisions produce a reactant only if the angle is appropriate.
- Reactions are reversible and they can experiment forward and reverse by selecting a different species to shoot.
- Students may describe things they discover about the reaction coordinate here too. See the note in #3

**4. Students will describe what would enable a reaction proceed or slow its progress with references to the reaction coordinate.**

- Based on the reaction coordinate and the energy of the reactants, students should be able to predict if a collision with a given energy will lead to products.
- For reactants that do not have enough energy to react, students should be able to propose how they could make the reaction happen through changes in temperature or use of a catalyst. They can't add anything that looks like a

catalyst, but they can change the activation energy by selecting Design your Own. Alternately, in order to stop a reaction from happening, they could propose how they could slow down or stop the reaction through changes in temperature or use of a catalyst.

- Reactions can proceed at lower temperatures if the activation energy is lowered. In a real reaction, this is done with catalyst.
- For the reaction to occur, reactant molecules must have sufficient energy to overcome the activation energy. Heating and cooling molecules will change their energy, and as a result will change the probability of successful collisions.

**5. Students will use the potential energy diagram to determine**

- The activation energy for the forward and reverse reactions,
- The difference in energy between reactants and products.
- The relative potential energies of the molecules at different positions on a reaction coordinate

**6. The reaction coordinate shows how potential energy changes with the separation of reactants and products.**

- The reaction coordinate shows the relative potential energies of the reactants, products, and the transition state.
- Different chemical reactions will have different reaction coordinates.

Second Panel, Many Collisions

**1. Describe reactions in terms of molecular models with illustrations.**

- The description should include: A chemical reaction given in the form  $A+BC \leftrightarrow AB+C$  or  $AB+CD \leftrightarrow AD+CB$  represents a large number of particles colliding and reorganizing to make new substances; Not every collisions results in a reaction; reactions are reversible.

**2. Use the molecular model to explain why reactions are not instantaneous.**

*Reactions are the result of collisions and that takes time. They may observe that rates vary, but since I don't plan to have them open the Reaction coordinate, they may not have an explanation for the observations.*

**3. Use the molecular model to explain why reactions have less than 100% yields.**

*Since reactions are reversible, even though products are being formed, they are reacting to make reactants, so there may not be 100% yield. We will have done a lab where they make rice crispy bars and I want to make sure that their explanations include more than a physical explanation that some reactants may stick to the container and not be able to collide. They may observe that rates vary, but since I don't plan to have them open the Reaction coordinate, they may not have an explanation for the observations.*

**3. Students will sketch how the number of reactants and products will change as a reaction proceeds**

- 4. Students will be able to determine the number of reactants or products from the experiment graph.**
- 5. Convert number to concentration**
  - Estimate the size of the container from the number of atoms across a side. Make an assumption for the depth of the container, the only parameter of the volume that isn't visible. From your estimate of the volume, and the number of atoms or molecules present, calculate the concentration.
- 6. Students will relate changes observed in the rate of reaction for a system of many molecules to changes at the molecular level, such as changes in the energy of molecules, or in the potential energy along the reaction coordinate.**
  - Just as heating and cooling will change the probability of a single reaction happening, heating and cooling will change the rate at which multiple reactant molecules proceed to form products.

**Equilibrium concepts that could be achieved in either the second or third panel:**

- 1. Students will explain how they know that a system has reached equilibrium from a graph of number of reactants and products versus time.**
- 2. Students will predict how raising or lowering the temperature will affect a system in the equilibrium position.**
- 3. Students will describe the relative sizes of the forward and reverse rates at equilibrium.**
- 4. Students will explain what effects whether the equilibrium position favors the products or the reactants.**
- 5. Students can predict how addition of a reactant or product will affect the forward and reverse reaction rates, and once this new system reaches equilibrium how the reactant and product concentrations will compare to the original system at equilibrium.**