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Supplementary material

SUPPLEMENTARY MATERIAL TO

Effect of simulations enhanced with conceptual change texts on university students' understanding of chemical equilibrium

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THE AREAS EVALUATED IN THE TESTS AND SOME OF THE TEST QUESTIONS

1. The following hypothetical reaction reaches equilibrium at 25ºC**:**

$$A_{(g)} + B_{(g)} \rightleftharpoons C_{(g)} + D_{(g)}$$

Once equilibrium has been reached, the concentration of C is increased by the addition of more C. Assume that the temperature remains constant. Which of the following can be said about the numerical value of the equilibrium constant?

(a) decreases (b) increases (c) *remains unchanged

Reason

(1) the rate of reverse reaction increases and the rate of the forward reaction decreases

(2) the rate of reverse reaction increases and the rate of forward reaction stays the same

(3) *the ratio between products' concentrations and reactants' concentrations is constant at constant temperature

(4) the concentration of the products has been increased

12. If you have a 0.5 M solution of sodium dichromate ($Na_2Cr_2O_7$) in which the following equilibrium is established

$$\underset{\text{yellow}}{2CrO_4^{2-}{}_{(aq)}} + 2H^+_{(aq)} \rightleftharpoons \underset{\text{orange}}{Cr_2O_7^{2-}{}_{(aq)}} + H_2O_{(l)}$$

and you add 10 mL of 0.5 M solution of sodium dichromate to the original solution what would you observe?

(a) the solution becomes yellow

(b) the solution becomes deeper orange

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(c) *the solution remains unchanged

Reason

(1) to counteract the increased amount of $Cr_2O_7^{2-}{}_{(aq)}$ the system will form more $CrO_4^{2-}{}_{(aq)}$

(2) there will be more collisions between particles of $Cr_2O_7^{2-}{}_{(aq)}$ and $H_2O_{(l)}$

(3) *there is no change in the concentration of any species

(4) because of increase in $Cr_2O_7^{2-}$, Q will be greater than K_{eq}

* Indicates the correct response

TABLE S-I. Characteristics of the CECT

Areas evaluated	Approach to equilibrium: items 3, 7, 8, 17 and 20
	Application of Le Chatelier's principle: items 4, 12, 13, 15 and 19
	Constancy of equilibrium constant: items 1, 5, 11, 14 and 16
	Heterogeneous equilibrium: items 2, 9 and 18
	Effect of a catalyst: items 6 and 10
Number of items	20
Response format	Two-tier multiple-choice
	First tier: content knowledge
	Second tier: reason for the content response
Time to complete test	30 to 35 minutes
Discrimination indices	Mean range (items)
	0.475 0.30-0.39 (2)
	0.40-0.49 (8)
	0.50-0.59 (5)
	0.60-0.69 (3)
	0.70-0.79 (2)
Difficulty indices	Mean range
	0.44 0.20-0.29 (3)
	0.30-0.39 (3)
	0.40-0.49 (6)
	0.50-0.59 (4)
	0.60-0.69 (2)
	0.70-0.79 (1)
	0.80-0.89 (1)
Cronbach Alpha	0.80

An example of the CCT designed to challenge the alternative conceptions that "the rate of forward reaction is greater than the reverse reaction one" and "forward reaction goes to completion before the reverse reaction starts"

Approach to Equilibrium

Introduction: What do you think about the progression of forward and reverse reactions?

Some students generally believe that and *"the rate of forward reaction is greater* *than the reverse reaction rate*" and "*forward reaction goes to completion before the reverse reaction starts"*. In other words, students see reversibility as referring to something that moves forward and then backwards, rather like a car. **These views are incorrect.**

As the reaction proceeds and the concentrations of reactants diminish, the rate of the forward reaction decreases. Namely, the reactant molecules collide and form product molecules, so the reactant concentrations drop. The rate of the forward reaction gradually decreases because the likelihood of collisions between reactant molecules decreases as their concentrations decrease. At the start of the reaction, there are no products in the container, so the rate of the reverse reaction is initially zero. But, as the concentrations of products increase, the rate of the reverse reaction increases. As the molecules of products form, the likelihood of their colliding with one another to reform reactant molecules increases and so does the rate of the reverse reaction. At a certain time, the reverse rate equals the forward rate and the equilibrium is achieved. As long as the rate of the forward reaction is greater than the rate of the reverse reaction, the concentrations of the reactants will steadily decrease, and the concentrations of products will constantly increase. These changes lead to a decrease in the rate of the forward reaction and an increase in the rate of the reverse reaction. This process continues until the two rates become equal. At this point, system has reached a dynamic equilibrium.

In a dynamic equilibrium for a reversible chemical reaction, the forward and reverse reaction rates are equal, so although reactants and products are constantly changing back and forth, there is no net change in the amount of either. Note that although the concentrations of reactants and products become constant, they do not become equal. As long as the system remains in a dynamic equilibrium, the concentrations of reactants and products remain constant, and the rates of the forward and reverse reactions also remain constant and equal. As a result, **the rate of forward reaction is greater than the reverse reaction one <u>until the equilibrium is established</u>.** At the equilibrium the rates of both reactions become equal.

On the other hand, some students believe that *forward reaction goes to completion before the reverse reaction starts.* **This is also incorrect**. If forward reaction goes to completion, concentration of at least one of the reactants becomes zero at the end of the reaction. This means that equilibrium constant will be unlimited and this is impossible. For example, let's consider the following reaction: $A + B \rightleftharpoons C + D$. If the forward reaction is completed, the concentration of A or B or both of them will become zero. The equilibrium constant of the reaction is $K_{eq} = [C][D] / [A][B]$. If the concentration of reactant(s) become zero the value of equilibrium constant will be unlimited. We know that all of the equilibrium reactions have a definite value of equilibrium constant. This means that both reactants and products have definite concentrations that are different from zero. **This show that forward reaction does not go to completion before the reverse reaction starts and both of them proceed until and during the equilibrium.**

TABLE S-II. Percentages of students' alternative conceptions in pre-test, post- and delayed-test; Pr-T: pre-test; Ps-T: post-test; D-T: delayed-test; CC: conceptual change; R: retention; NR: non-retain; +: positive conceptual change

Alternative conceptions		Experimental group					Control group				
		Pr-T	Ps-T	D-T	CC	R	Pr-T	Ps-T	D-T	CC	R
Approach to equilibrium	Forward reaction goes to completion before the reverse reaction starts	70	13	28	+57	NR	68	50	57	+18	NR
	Concentration of reactants equal the concentration of products at equilibrium	48	24	24	+24	R	48	37	53	+11	NR
	The rate of forward react-ion is always greater than the reverse reaction one	66	17	24	+49	NR	64	43	57	+21	NR
	The rate of the reaction increases until equilibrium is established	56	23	22	+33	R	57	47	43	+10	R
	The rate of the forward reaction increases with time and that of the reverse reaction decreases until the equilibrium is reached	48	23	23	+25	R	58	40	41	+18	NR
	The forward reaction com-plete before the reverse reaction complete	66	35	34	+31	R	61	37	42	+24	NR
	At equilibrium system, moles equal concentrations in any species	58	41	45	+17	NR	59	48	57	+11	NR
	At equilibrium, no reaction occurs	56	24	24	+32	R	58	40	43	+18	NR
Application of Le Chat-elier's principle	Le Chatelier's principle can be applied in the initial state before the reaction has reached equilibrium	66	29	29	+37	R	64	43	57	+21	NR
	When the temperature is changed, the type of react-ion (endothermic or exo-thermic) does not affect the direction of the equilibrium shift	58	28	28	+30	R	65	50	60	+15	NR
Application of Le Chat-elier's principle	When a substance is added to equilibrium mixture, equilibrium will shift to the side of addition	56	28	27	+28	R	64	40	50	+14	NR
	Increasing the temperature of an exothermic reaction would decrease the rate of the forward reaction	52	24	24	+28	R	58	39	49	+19	NR

TABLE S-II. Continued

Alternative conceptions		Experimental group					Control group				
		Pr-T	Ps-T	D-T	CC	R	Pr-T	Ps-T	D-T	CC	R
Application of Le Chatelier's principle	When the temperature is increased, more products are formed	62	29	29	+33	R	62	37	53	+25	NR
Constancy of equilibrium constant	An increase in temperature always increases the numerical value of K_{eq}	59	24	30	+25	NR	57	43	51	+14	NR
	Equilibrium constant, K_{eq}, will increase with increasing temperature in an exothermic reaction	65	35	35	+30	R	61	46	52	+15	NR
	Large values of equilibrium constant imply a very fast reaction	51	28	27	+23	R	62	42	47	+20	NR
	When more reactants are added to an equilibrium system, Keq will change	53	24	24	+29	R	59	36	47	+23	NR
	When more products are added to an equilibrium system at constant temperature, K_{eq} will increase	64	35	35	+29	R	65	46	50	+19	NR
	The numerical value of K_{eq} changes with the amounts of reactants or products	56	24	23	+32	R	59	47	53	+12	NR
Heterogeneous equilibrium	Le Chatelier's principle can be applied in all systems, including heterogeneous equilibrium systems	65	31	31	+34	R	65	43	57	+22	NR
	When a solid substance is added to an equilibrium system at constant temperature, Keq will change	60	28	28	+32	R	60	37	45	+23	NR
Effect of a catalyst	The rate of the forward and reverse reactions could be affected differently by addition of a catalyst	64	13	12	+51	R	57	35	43	+22	NR
	Catalyst increases the value of equilibrium constant	47	17	20	+30	NR	50	28	36	+22	NR
Reversible and non-reversible reaction	A reversible reaction goes to completion	46	23	23	+23	R	55	34	42	+21	NR