

Acid-Base Solutions

PhET Sim design document

version 0.5

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public URL: http://docs.google.com/Doc?id=dfnd4k2x_83gx2cgsd7

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Recent Changes

- Jan 16 (Archie)
 - new [mockup](#) for tab 4
- Jan 15 (Archie)
 - new design and [mockup](#) for reaction equation resizing
 - new design and [mockups](#) for tab 3 (Matching Game)
- Jan 13 (Archie)
 - new [mockup](#) for tab 2 with bar graphs
 - $K_a \rightarrow K_a$ (and $K_b \rightarrow K_b$)
- Jan 12, 2009 (Archie)
 - new [mockup](#) for custom weak base
 - new [mockup](#) for "view symbol legend"
 - included email discussion in [Comments&Discussion](#) for posterity
 - added section for the [model](#)
- Jan 7, 2009 (Archie)
 - changed to version 0.5
 - new "Comparing Solutions" tab
 - new "Symbol Legend" button and window
 - Laurie's general learning objectives added to learning goals
 - bar charts: changed order of bars and graph label
 - logarithmic concentration slider
 - Lewis structures shown in "View Reaction Equations"
- Dec 19 (Archie, following meeting with Kathy and Trish)
 - changed to version 0.4
 - intro and advanced tabs merged
 - new "Matching Game" tab (incomplete)
 - long list of chemicals ([here](#))
- Dec 15 (Archie, following design meeting of Dec 12)
 - changed version to 0.3
 - new name for sim

- now has three tabs
 - some layout changes
- Dec 9 (Archie)
 - changed version to 0.2
 - included K_a on pH meter
 - included Molecule Count view
 - included custom option for acids and bases
 - added molecule icons
 - added reaction equations
- Dec 4, 2008 (Archie)
 - document started, version 0.1
 - split from second tab of "Modelling Water, Acids & Bases" sim design document

Note: previous versions may be viewed from the Google Docs "File" menu, under "Revision History" (when this document is in edit mode).

Outstanding Issues

The following issues require action by the design team.

Higher priority:

1. Are we satisfied with the appearance of the variable symbol size in the "View reaction equations" window? (see [mockup](#))
2. [Learning goals](#) should be edited by Laurie.
3. Need second opinions on design of tabs 3 and 4.

Lower priority:

1. What text should be included in the symbol legend window? (see [mockup](#))
2. Are the fonts too small in the bar graphs for the second tab? (see [mockup](#))
3. What should the "View" checkboxes say for tab 2? The label must accommodate having an acid in one beaker and a base in the other (see [mockup](#)).
4. Issues remain on specifics in the [model](#) . (See '??' marks in that section.)
5. Need to choose which chemicals to include from the [list](#). We should be sure that all are realistic -- for instance, can we even have an 8 M solution of HCN?
6. How can we make the concentration scale more easy to interpret (add more labels)?
7. What range of concentrations should we allow?
8. Colors need to be decided on.
9. We need usage scenarios once we settle on the learning goals.

Learning Goals

Students will be able to...

1. describe the similarities and differences between
 - strong acids and weak acids.
 - strong bases and weak bases.
 - strong acids and strong bases.
 - weak acids and weak bases.
2. describe the similarities and differences between concentrated and dilute solutions.
3. describe what it means if you have a
 - concentrated solution of a weak acid (or base).
 - concentrated solution of a strong acid (or base).
 - dilute solution of a weak acid (or base).
 - dilute solution of a strong acid (or base).
4. calculate concentration of acid (or base) given the concentrations of their components in solution.
5. calculate percent dissociation of an acid (or base) from their component concentrations.
6. relate the percent dissociation to the strength of acid (or base).
7. determine or predict the concentrations of water and acid (or base) components in solution
 - knowing percent dissociation
 - knowing ...?
8. identify whether certain common chemicals are strong or weak (chemicals given in drop-down).
9. identify the generalized symbols for acids (HA) and bases (B or MOH).

Objectives for student learning from sim:

Laurie composed the following general objectives that the sim should meet, not necessarily in the form of learning goals.

1. Students should develop a sense of what "strength" means in terms of acids and bases.
2. Students should develop a sense of what "concentration" means in terms of acid and base solutions.
3. Students should understand how strength and concentration together affect pH, percent dissociation, and concentrations of ions in solution.
4. Students should be able to predict all chemical species that will be in a particular acid or base solution, and identify what the major and minor species are.
5. Students should be able to use and produce multiple representations that describe what's happening and what's present in a particular acid or base solution. These representations include: bar graphs showing all solution components, beaker view / dot view, chemical equations (using chemical symbols, equilibrium or non-equilibrium arrows), K_a/K_b values, K_a/K_b expressions, specialized symbols (K_a , K_b , HA, A⁻, B, BH⁺), and Lewis structures.
6. Students should be able to describe what makes something an acid or a base (using pH values, chemical equations showing whether H₃O⁺ or OH⁻ are produced, etc.)

Laurie says: Embedded within many of these learning goals is being able to qualitatively describe effects of strength and/or concentration on pH, percent dissociation, and concentrations of species in solution, as well as to calculate pH, percent dissociation, and concentrations of species in solution.

Basic Sim Operation

Briefly, overall:

- first tab ("Solutions")
 - select a solution of weak or strong acid or base
 - change the concentration of the solution with a slider
 - observe (with 'dot view' or by bar graph) the concentrations of the various components
- second tab ("Comparing Solutions")
 - two controllable solutions are shown, so user can compare them
 - essentially two instances of the contents of the first tab
- third tab ("Matching Game")
 - game with points given for matching a solution with an unknown solution
 - the user first decides if it's an acid or base, then if it's weak or strong
 - the user then manipulates the concentration and strength of the solution in the second beaker to match the first
- fourth tab ("Find the Unknown")
 - like the first tab, except that the user chooses the chemical in two drop-downs (one to pick which unknown, the second to choose from a variety of unknown solutions)
 - also, one of the display elements is replaced by a "?" which is derivable from the other data shown

First Tab ("Solutions")

- see [mockup](#)
- Bar graphs
 - not controllable
 - can be minimized by clicking the X in the upper right
 - when minimized, the graph is replaced by a button (similar to "View Reaction Equations") that says "View Concentration Graphs"
 - shows HA/A⁻ bars if a custom/generic acid is in the beaker
 - shows B/BH⁺ bars if a custom weak base is in the beaker (see [mockup](#))
 - shows MOH/M⁺ bars if a generic strong base is in the beaker
 - shows true chemical symbols if a real (not custom) chemical is in the beaker
 - some chemical symbols are long; these labels may have to be angled to fit (see [mockup](#))
- Beaker
 - in default (start up) state, there is no acid or base
 - contains 1 liter volume (not changeable)
 - can show dots
 - controlled by "View box" (see below)
 - show either:
 - ratios of hydronium/hydroxide
 - HA/A⁻ (or B/BH⁺ if bases are selected)
- "View" box (by beaker)
 - ratio check boxes (see [mockup](#))

- can select to see either or both
 - dots for hydronium and hydroxide
 - dots for dissociated acid (or base) components
 - the labels for the middle line will change according to what's in the beaker:
 - for acids, HA/A^- ratio
 - for bases, B/BH^+ ratio
 - true chemical symbols if a real (not custom) chemical is in the beaker (eg, HCl, HCl/Cl⁻ ratio, etc)
 - "Molecule Count" check box (see [mockup](#))
 - when checked, show a display of total numbers of molecules of each type in the bar chart (similar to pH Scale feature)
- pH readout
 - shows pH of solution
 - not controllable
- "View Reaction Equations" button
 - pops up a separate window that shows reaction equations (not controllable); see [mockup](#)
 - if the window is already open, clicking the button will change focus to that window
 - window shows three equations
 - one of the following (along with Lewis structures):
 - $\text{HA} + \text{H}_2\text{O} \leftrightarrow \text{H}_3\text{O}^+ + \text{A}^-$ if there's an acid in the beaker
 - $\text{B} + \text{H}_2\text{O} \leftrightarrow \text{OH}^- + \text{BH}^+$ if there's a base in the beaker
 - similar equation with correct chemical symbols (for a real chemical)
 - $\text{H}_2\text{O} + \text{H}_2\text{O} \leftrightarrow \text{H}_3\text{O}^+ + \text{OH}^-$ (along with Lewis structures)
 - the equation to calculate K_a (or K_b for bases)
 - notes on equations:
 - the "A" and "B" are replaced by the correct chemical symbols if a real (not custom or generic) chemical is in the beaker
 - if the acid or base is strong, the second equation has a right arrow rather than the double arrow in the equation
 - resizing of symbols in equations
 - the radio button in the "View" window defaults to 'off', in which case the symbols in the equations remain static (see [mockup](#))
 - if the radio button is turned 'on', the sizes of all chemical symbols except for H_2O will vary with their concentration in solution (see [mockup](#))
 - the relation that governs the font size in the [mockup](#) is a quadratic function of the log of the molecule's concentration (this relation will be included here if the design team agrees on its appearance)
- "View Symbol Legend" button
 - see [mockup](#)
 - pops up a separate window with text that shows what symbols mean (not controllable)
 - if the window is already open, clicking the button will change focus to that window
 - window shows:
 - (to be determined)
- "Show/Hide K_a " button
 - Shows the K_a value in the "Solution" box when selected
 - Text changes to "Hide K_a " if K_a is being shown
 - default state is hiding K_a display
 - text should change to K_b if a base is in the solution
- "Solution" control box
 - choices in drop-down (ordered):
 - Pure Water
 - Generic Strong Acid (HA)
 - Custom Weak Acid (HA)
 - Generic Strong Base (MOH)
 - Custom Weak Base (B)
 - Acetic acid (CH_3COOH)
 - Ammonia (NH_3)
 - Hydrochloric acid (HCl)
 - Hydrocyanic acid (HCN)
 - Perchloric acid (HClO_4)
 - Potassium hydroxide (KOH)
 - Pyridine ($\text{C}_5\text{H}_5\text{N}$)
 - Sodium hydroxide (NaOH)
 - strength slider

- controls the strength of the acid base only if a "custom weak" acid or base is selected (is greyed out otherwise)
- if a weak acid/base is selected (but not "custom"), the pointer will show its strength but will not be adjustable (see [mockup](#))
- if a strong acid/base is selected, the slider will disappear and the word "Strong" will appear on the slider (see [mockup](#))
- label changes from "Acid Strength" to "Base Strength" if there's a base in the solution
- concentration slider
 - will change the concentration of the acid/base in solution
 - label changes from "Acid Concentration" to "Base Concentration" according to what's in solution
 - goes logarithmically from 0.001 to 8 Mol/L
 - bar graph and dots will change accordingly
- concentration textbox
 - shows value of concentration slider (3 decimal places)
 - editable (from 0.001-8)
- K_a/K_b readout:
 - not shown by default
 - only shown when "Show K_a " button is selected
 - not adjustable
 - shows value of the acid's K_a , or the base's K_b ($K_a = [H_3O^+][A^-]/[HA]$)
 - if a strong acid/base is selected, readout just says "Large"

Second Tab ("Compare Solutions")

- two controllable solutions (as in tab 1), one in left and one in right panel
- variable view type (view is the same for both panels); can be:
 - beakers (see [mockup](#))
 - sub-menu with check boxes for dots and/or molecule count
 - label for dots view will have to be something that can accommodate both acid and base (currently "chemical ion ratio")
 - bar graphs (see [mockup](#))
 - bar graphs will have to be slightly reduced in size compared to tab 1, otherwise they are equivalent
 - equations
 - shows the same content as in the "View Reaction Equations" window in each panel
 - will have to be scaled down so that they fit

Third Tab ("Matching Game")

- a game with points to control a solution in the right panel until it matches the one presented in the left panel
- start-up state (Question 1)
 - see [mockup](#)
 - a solution is chosen at random and shown in the left panel
 - the "dots" for the H_3O^+/OH^- ratio are shown, other view options are greyed out
 - a "wiggle-me" appears with very basic game instructions (red text in [mockup](#))
 - the user must chose if it's an acid or base
 - correct choice leads to Question 2 (next bullet) and +1 point
 - incorrect choice leads to -1 point and "wrong" message
- Question 2
 - see [mockup](#)
 - appears when Question 1 has been answered correctly
 - view options are still greyed out
 - asks if it's weak or strong (uses the appropriate wording for "acid" or "base")
 - the user must chose if it's weak or strong
 - correct choice leads to Question 3 (next bullet) and +1 point
 - incorrect choice leads to -1 point and "wrong" message (see [mockup](#))
- Question 3
 - see [mockup](#)
 - appears when Question 2 has been answered correctly
 - all view options are available
 - same options as in tab 2, except there is no "equations" option
 - pH readout becomes visible
 - more controls now available
 - uses the appropriate wording for "acid" or "base"
 - user may now control the concentration by slider
 - user may control strength only if this is a weak acid/base
 - for strong acid/base, slider displays "Strong" as in first tab
 - weak/strong is a radio button that may be changed
 - the user can change setting with no point changes until "check match" button is clicked, then
 - if the two solutions are sufficiently close:

- +1 point
 - "Correct!" message
 - user must click "next solution" to continue
- incorrect choice leads to -1 point and "wrong" message
- user can at any time click "next solution" button, then
 - "number of solutions" readout will increment by one
 - a new solution is chosen and the display goes to start-up state
- "reset all"
 - changes "points" and "number of solutions" back to zero
 - display goes to start-up state

Fourth Tab ("Find The Unknown")

- see [mockup](#)
- looks the same as the first tab, except for
 - "solutions" control box has no sliders and two drop-down menus
 - certain display elements will be erased and replaced with a "?", depending on drop-down choices
- first drop-down menu ("choose the unknown")
 - find pH
 - pH meter readout replaced with "?"
 - find K_a (or K_b)
 - K_a/K_b meter readout replaced with "?"
 - find the H_3O^+ and OH^- concentrations
 - two bars and concentration readout replaced with "?"
 - find the HA and A⁻ concentrations (or B, BH⁺)
 - two bars and concentration readout replaced with "?"
- second drop-down menu ("choose the solution")
 - options are "Solution X", "Solution Y", etc
 - has a different set of solutions for each option in the first drop-down

Model

The following describes the mathematical model governing all quantities in the sim.

- relations & notation (common to all calculations)
 - constants
 - $A = 6.022e23$ (Avogadro's number, 1/mol)
 - $W = 55.56$ (concentration of pure water, mol/L)
 - independent variables
 - c = concentration (mol/L)
 - set by user, ranges from $1e-3$ to 8
 - K_a = strength of weak acid (mol/L)
 - set by user, ranges from $1e-12$ to $1e-2$ (??) or by chemical type (see [table](#))
 - K_b = strength of weak base (mol/L)
 - set by user, ranges from $1e-12$ to $1e-2$ (??) or by chemical type (see [table](#))
 - p = percent ionization (no units)
 - $[x]$ = concentration of molecule x (mol/L)
 - $pH = -\log_{10}([H_3O^+])$
 - number of molecules of $x = [x] \cdot A$
- Strong Acid
 - $[HA] = 0$
 - $[A^-] = c$
 - $[H_3O^+] = c$
 - $[OH^-] = 1e-14 / c$
 - $[H_2O] = W - c$
 - $p = 100$
- Strong Base
 - $[MOH] = 0$
 - $[M^+] = c$
 - $[OH^-] = c$
 - $[H_3O^+] = 1e-14 / c$
 - $[H_2O] = W$ (??)

- $p = 100$
- Weak Acid
 - $[A^-] = (-K_a + \sqrt{K_a^2 + 4 * K_a * c}) / 2$
 - $[H_3O^+] = [A^-]$
 - $[HA] = c - [A^-]$
 - $[OH^-] = 1e-14 / [A^-]$
 - $[H_2O] = W - [A^-]$
 - $p = 100 * [A^-] / c$
- Weak Base
 - $[BH^+] = ??$
 - $[H_3O^+] = ??$
 - $[B] = ??$
 - $[OH^-] = ??$
 - $[H_2O] = ??$
 - $p = ??$

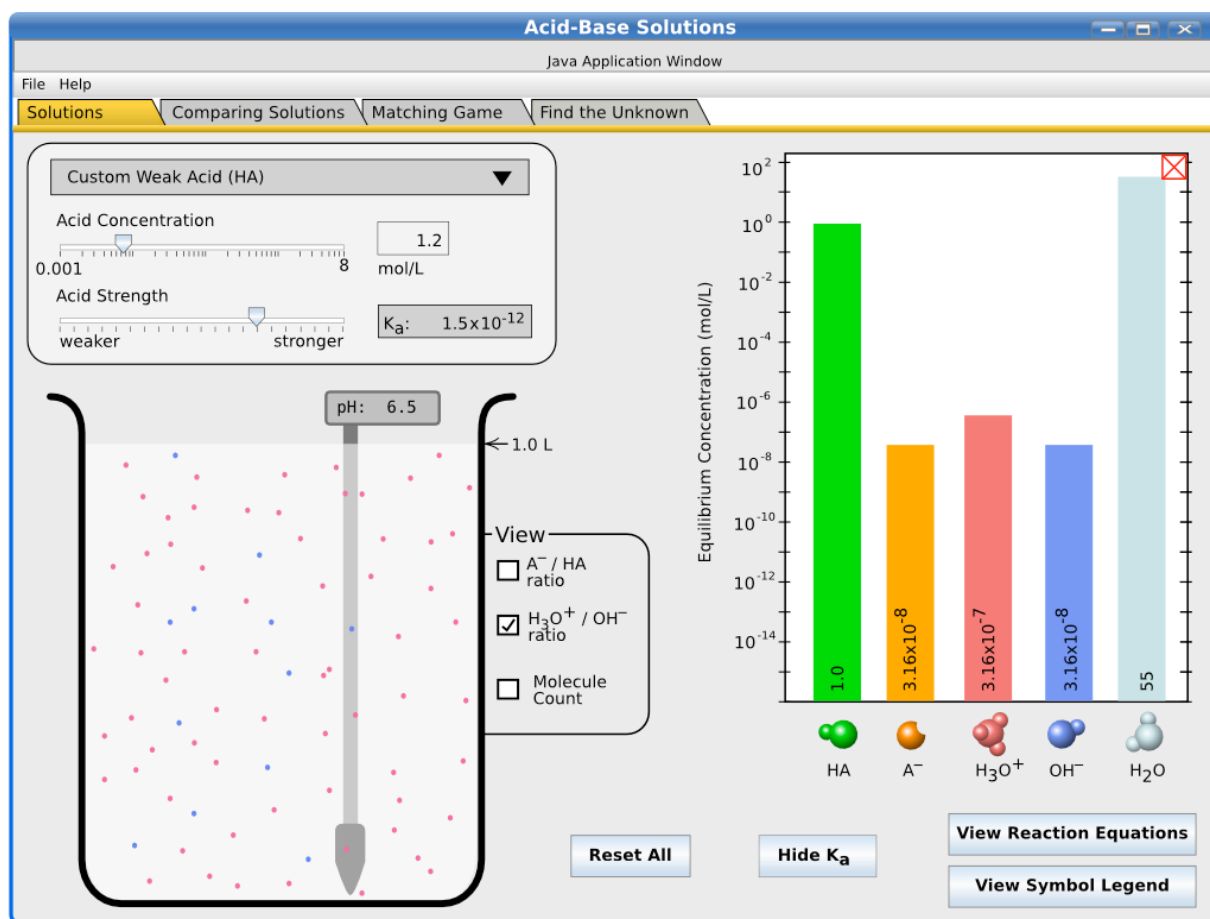
Usage Scenarios

We need usage scenarios illustrating how we hope users will interact with this sim. Scenarios should be linked to the learning goals.

Mockups

Note: all quantitative values in the mockups are bogus placeholders.

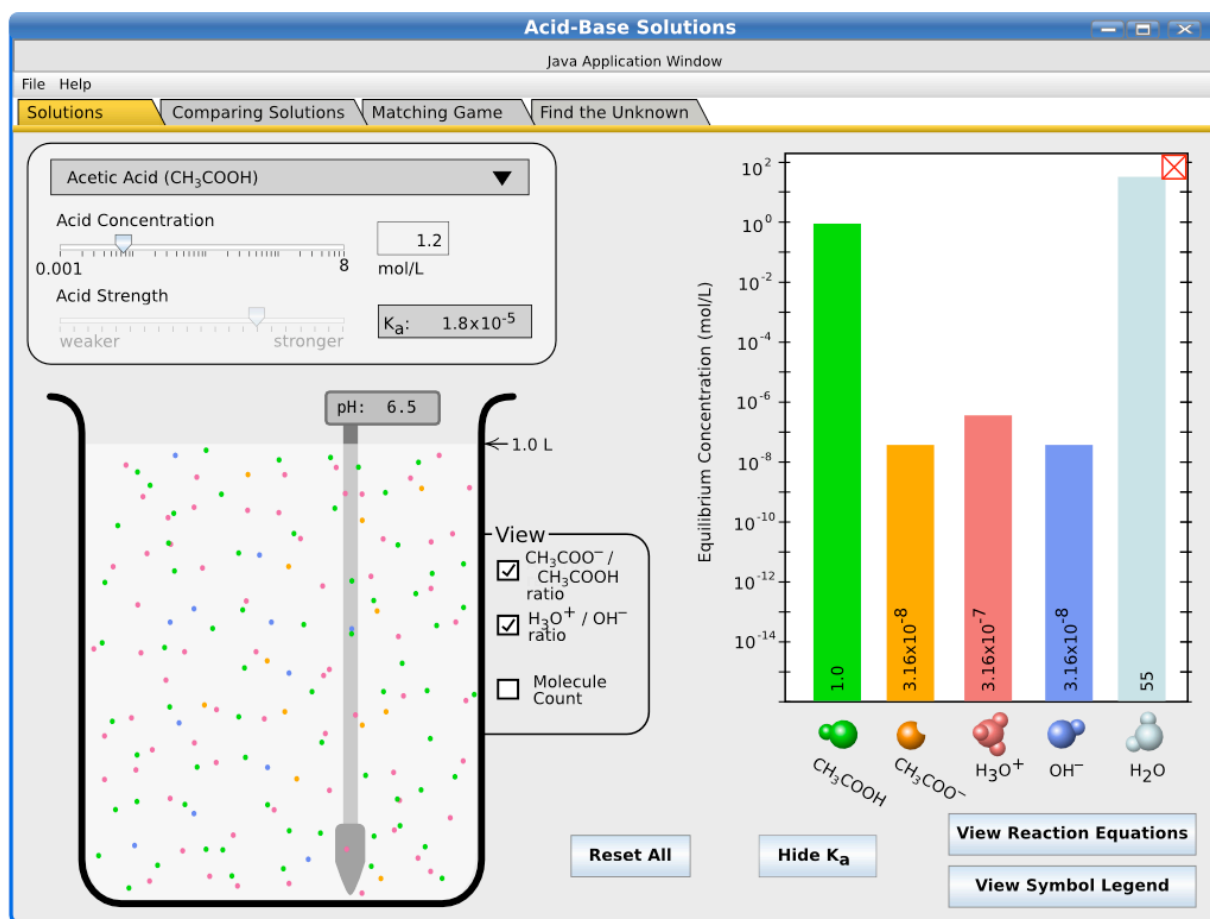
First Tab ("Solutions"):



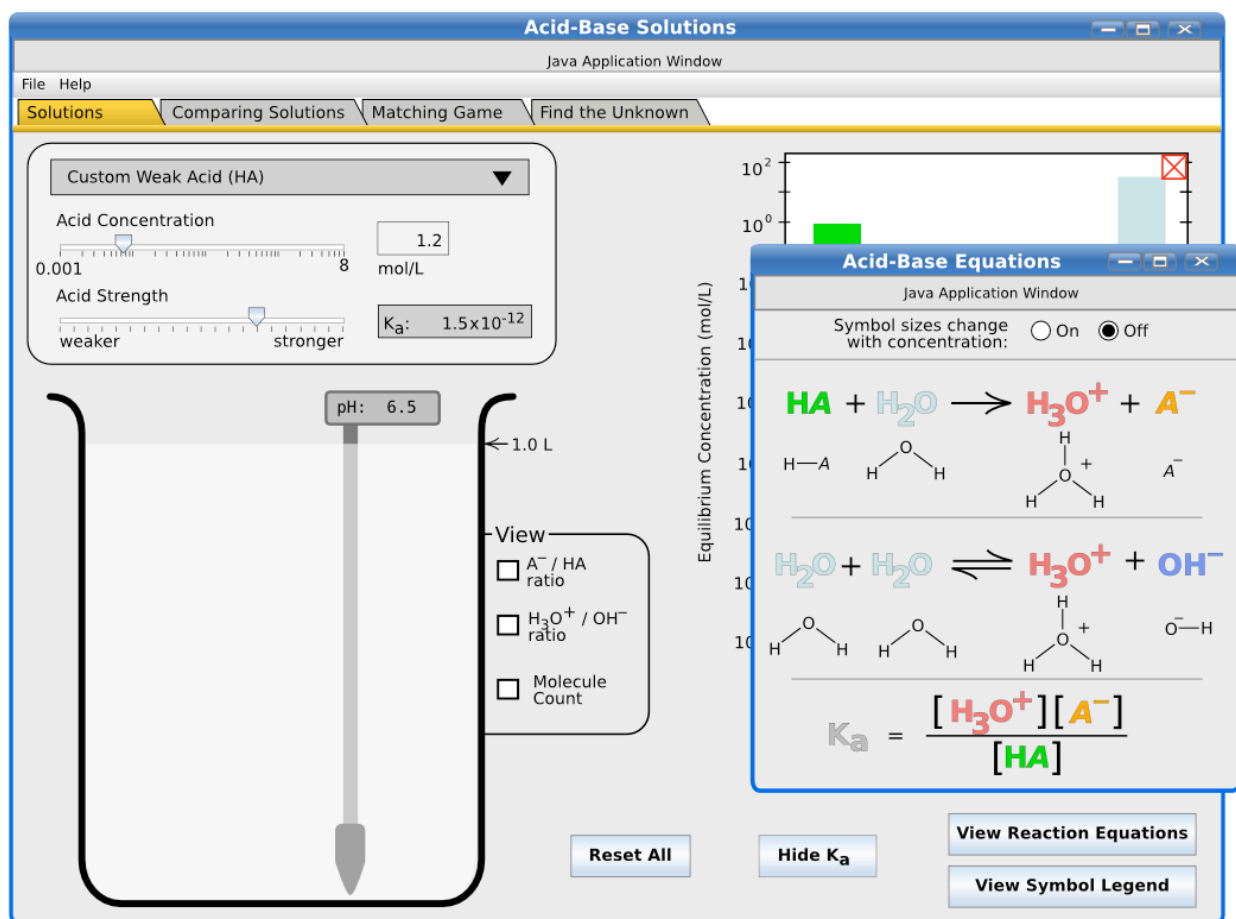
First Tab variant with "Hydrochloric Acid" and "Molecule Count" selected:



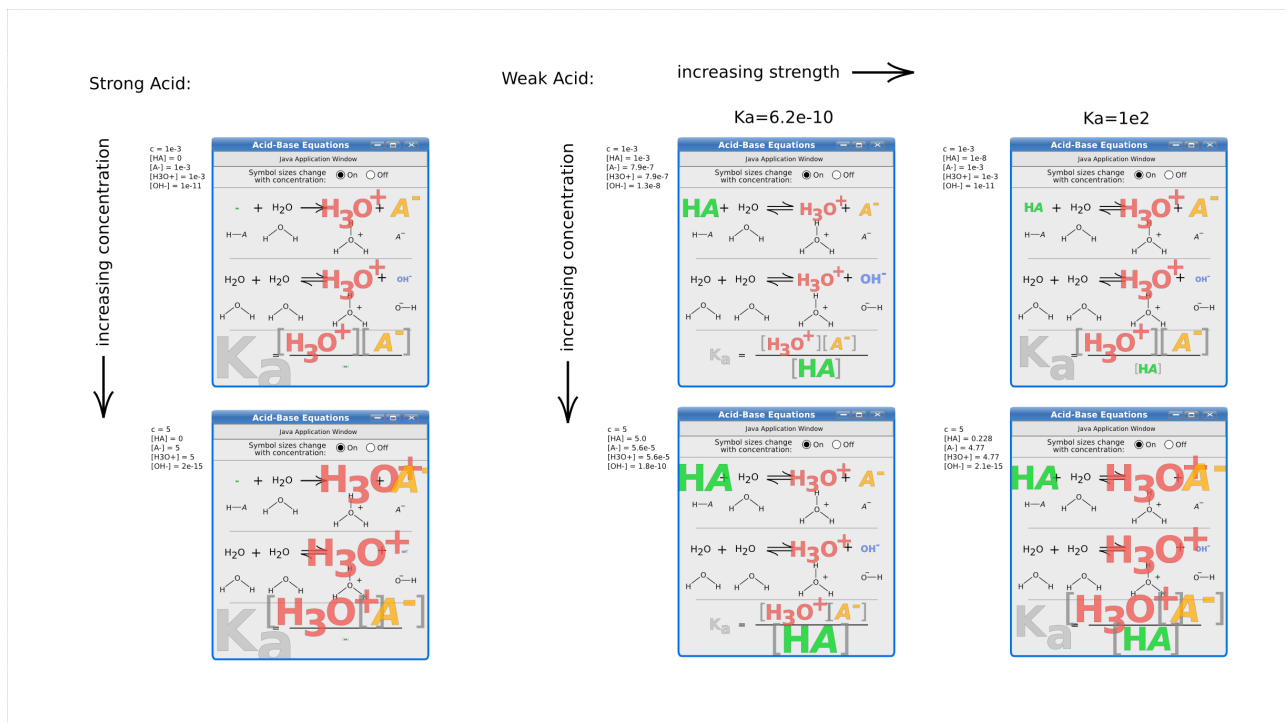
First Tab variant with "Acetic Acid" and all dots selected:



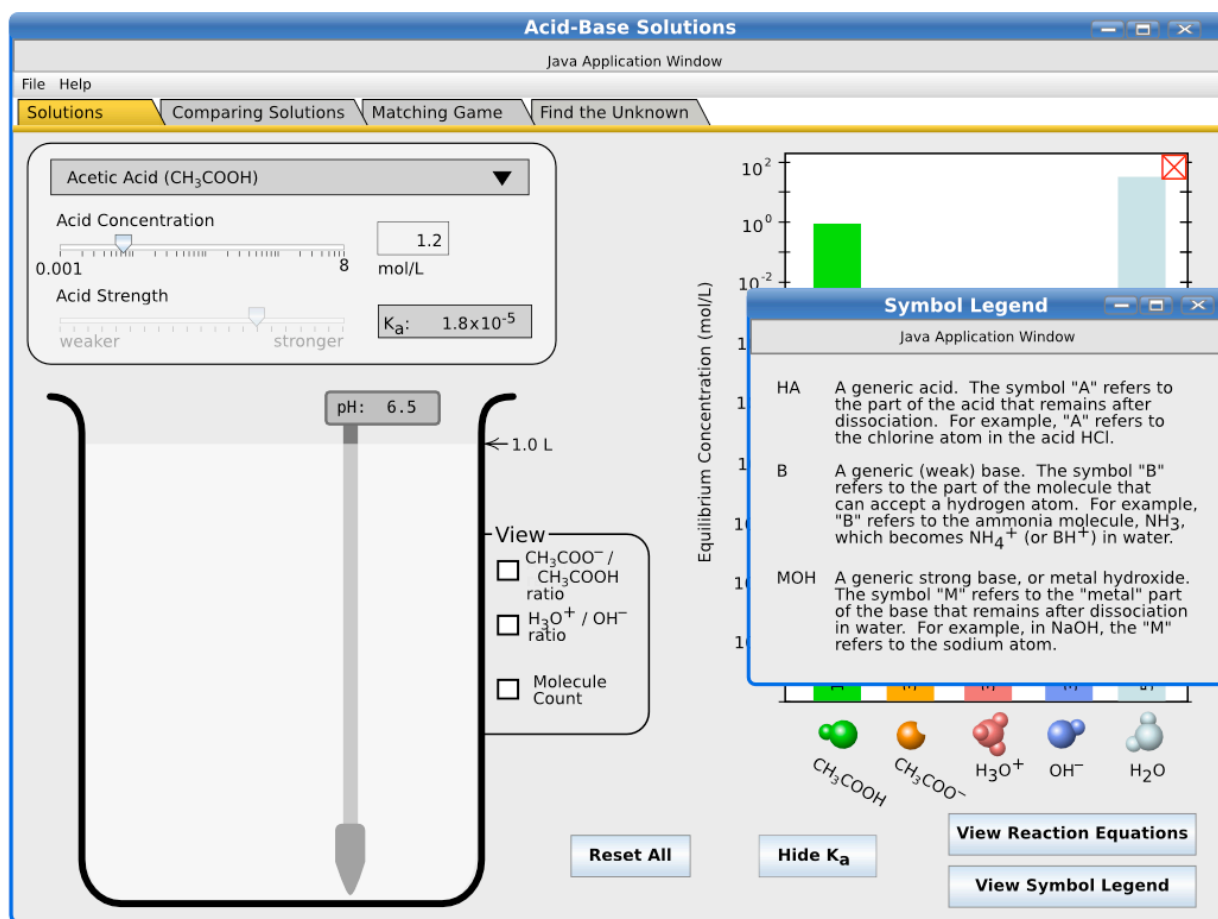
First Tab with View Reaction Equations Window:



Reaction equations resizing (click image for larger version):



View Symbol Legend Window:



Second Tab ("Compare Solutions"):

Acid-Base Solutions

Java Application Window

File Help

Solutions Comparing Solutions Matching Game Find the Unknown

Custom Weak Acid (HA)

Acid Concentration 1.2 mol/L

Acid Strength $K_a: 1.5 \times 10^{-12}$

Custom Weak Base (B)

Base Concentration 1.2 mol/L

Base Strength $K_b: 1.5 \times 10^{-12}$

pH: 6.5

View

- ☒ Beaker
- ☐ chemical ion ratio
- ☒ H_3O^+ / OH^- ratio
- ☐ Molecule Count
- ☐ Bar Graphs
- ☐ Equations

Reset All

← 1.0 L

Second Tab with "Bar Graphs" selected:



Third Tab ("Matching Game") initial state:

Acid-Base Solutions

Java Application Window

File Help

Solutions Comparing Solutions Matching Game Find the Unknown

Points: 0

Number of Solutions: 0

Next Solution

Match this solution with this one using these controls

Is the solution an acid or a base?
Select one:
☐ Acid
☐ Base

pH: 6.5

View

- ☒ Beaker
- ☐ chemical ion ratio
- ☒ $\text{H}_3\text{O}^+/\text{OH}^-$ ratio
- ☐ Molecule Count
- ☐ Bar Graphs

Reset All

pH: ← 1.0 L

Third Tab after clicking "acid":

Acid-Base Solutions

Java Application Window

File Help

Solutions Comparing Solutions Matching Game Find the Unknown

Points: 1 **+1 point**

Number of Solutions: 0

Correct!

Next Solution

Is the solution a weak acid or a strong acid?
Select one:

☐ Weak
☐ Strong

View

☒ Beaker

☐ chemical ion ratio

☒ $\text{H}_3\text{O}^+/\text{OH}^-$ ratio

☐ Molecule Count

☐ Bar Graphs

Reset All

pH: 6.5

pH: ← 1.0 L

Third Tab after (incorrectly) clicking "strong":

Acid-Base Solutions

Java Application Window

File Help

Solutions Comparing Solutions Matching Game Find the Unknown

Points: 0 **-1 point**

Number of Solutions: 0

wrong

Next Solution

Is the solution a weak acid or a strong acid?
Select one:

☐ Weak
☐ Strong

pH: 6.5

View

☒ Beaker

☐ chemical ion ratio

☒ $\text{H}_3\text{O}^+/\text{OH}^-$ ratio

☐ Molecule Count

☐ Bar Graphs

Reset All

pH:

← 1.0 L

Third Tab after getting the first two questions correct:

Acid-Base Solutions

Java Application Window

File Help

Solutions Comparing Solutions Matching Game Find the Unknown

Points: 1

Number of Solutions: 0

Check Match

Next Solution

weak acid strong acid

Acid Concentration

0.001 8 mol/L

1.2

Acid Strength

weaker stronger

K_a : 1.5×10^{-12}

pH: 6.5

View

☒ Beaker

☐ chemical ion ratio

☒ H_3O^+ / OH^- ratio

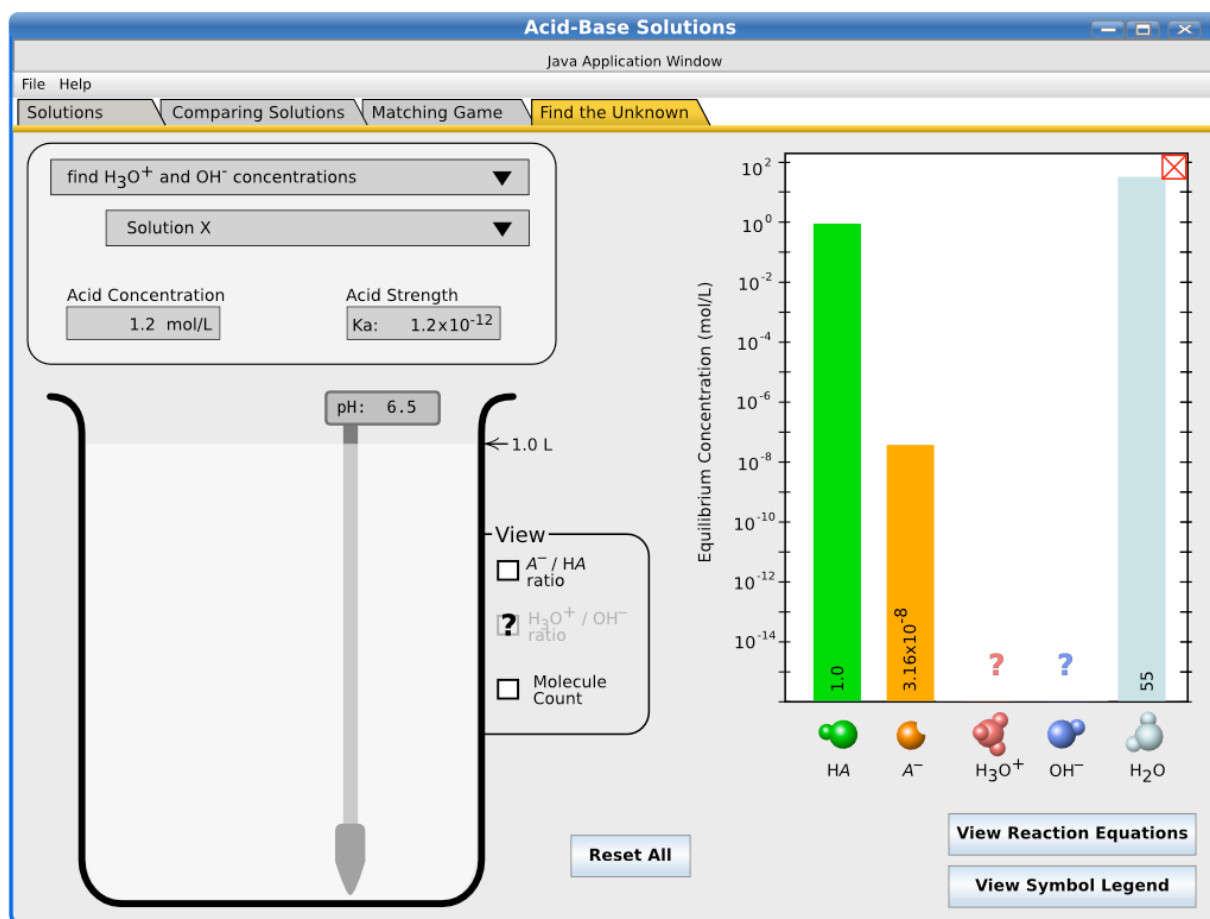
☐ Molecule Count

☐ Bar Graphs

Reset All

← 1.0 L

Fourth Tab ("Find The Unknown"):



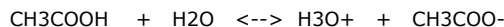
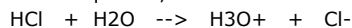
Comments and Discussion

Comments and responses by the design team in chronological order. Issues that still require attention are in the [Outstanding Issues](#) section.

Kathy's comments (Dec 8, 2008)

- I am thinking that it would be useful to import a few more things from pH scale ...
 - a readout for molecular counts (Archie says: done in design version 0.2.)
 - little icons representing the atoms / molecules. (Archie says: done in design version 0.2.)
 - ability to interact with HA (mol/L) on graph directly (Laurie says: I don't think this last point is necessarily important.)
- Ability to vary the strength of the acid from weak to strong dynamically in addition to allowing selection of strong or weak acid or base (so having a slider that allows you to do this). (This dynamic interaction is usually pretty powerful for learning and relating the differences). - so for instance keeping the acid concentration the same, but varying its strength and seeing what that means in terms of the HA and A^- concentrations.
 - Archie says: Now included in design version 0.2.
- I think we might want to bring in the additional connection to the equilibrium equation that students use in class: $\text{HA}(\text{aq}) + \text{H}_2\text{O}$ (arrows) $\text{H}_3\text{O}^+(\text{aq}) + \text{A}^-(\text{aq})$ $K_a = [\text{H}_3\text{O}^+][\text{A}^-] / [\text{HA}]$ So they can relate "strength" to these equations as well as to the visualization of what is in solution.
 - Archie says: An idea for this is shown in the mockup for design version 0.2.
 - Laurie says:
 - when dealing with strong acids, don't use equilibrium arrow. Just $\text{HA} + \text{H}_2\text{O} \rightarrow \text{H}_3\text{O}^+ + \text{A}^-$
 - It gets a little more complicated with strong bases as well. For the most part, the strong bases students will encounter in aqueous solutions are metal hydroxides. So, NaOH, $\text{Mg}(\text{OH})_2$, KOH . . . The "generic" way of representing this would be either $\text{MOH} \rightarrow \text{M}^+ + \text{OH}^-$ or $\text{M}(\text{OH})_2 \rightarrow \text{M}^{2+} + 2\text{OH}^-$
 - If students select a particular acid or base solution from the drop-down menu, I think it would be useful to show the

actual equation, so:



- o Archie says: included in version 0.3 ("view reaction equations" window)
- 4. Possible extension of this sim through the addition of a second panel which allows titrations/dilutions.
 - o this would allow you to have a faucet of neutral water that you can add.
 - o allow you to add small amounts of an acid or base
 - o setting the mol/L of what you add, the qualitative strength of what you add, and to control pretty well the volume of what you add
 - o this would add back in the ability to change the volume of the vessel [ie, the fluid]
 - o Trish says: adding a titration panel seems like a big project and I wonder if it should be a separate sim.
 - o Laurie says: Agree with Trish that titrations is a separate sim. Dilutions could be okay. I don't know if we'd want to do it "properly," that is, adding the concentrated acid to the water (instead of adding water to the acid--that's a real safety concern in lab. I know simulations aren't "real" but I'd hate to model unsafe lab practices anyway. There's a saying, "There she lies cold and placid, because she added water to the acid.") I think that for this sim, "diluting" using the existing slider is fine.
 - o These will not be implemented in this sim.
- 5. I could also envision a "find the unknown" game of sorts (different panel), where the teacher can make them do some calculations ...
 - o e.g. find the pH if we plot up the concentrations.
 - o or find the concentrations if they know the pH and the
 - o Laurie says: I think this as a second panel would be good. One possibility is this: Pull-down menu has "Solution A," "Solution B," "Solution K" etc. Students can change concentration. But, essentially, they get a readout of pH, and bar graphs of concentrations of species (could also have the dot views). The first-level question is "Is it an acid or base?" Then, by using concentrations and dot views to see whether it's completely dissociated, they can answer the second-level question of "Is it weak or strong?" If it's strong, they could suggest an identify. If it's weak, they can then use the concentrations of species to calculate K_a or K_b and then identify the acid or base that way. Another possibility would be a "predict the pH" unknown game. Here, students would control the strength (K_a or K_b) and concentration, then predict the pH by performing calculations. They could then turn on the pH meter to check their answer.
 - o Archie says: included in plans (version 0.3), but not completely designed yet
 - o Archie now says: design completed in version 0.5

Chris's comments (Dec 9, 2008)

1. Should the beaker have tick marks and labels, ala pH Scale?
 - o (Archie) not necessary since solution volume cannot change
2. The "dot view radio buttons" should be placed near the beaker (as in pH Scale). Putting them below the graph gives the erroneous impression that these controls pertain to the graph.
 - o (Archie) done in design version 0.2.

Laurie's comments (Dec 23, 2009)

1. Since many of the solutions we're dealing with are in an equilibrium state, would it be possible to have the dots moving in the beaker, and have a few change from HA to A⁻ and vice versa? Since students can't change the volume of the liquid, the number of dots at a given concentration will remain constant, so I hope it's feasible to add motion.
 - o Chris says:
 - implementation issues: requires adaptation of the ph-scale code, instead of direct reuse; requires a model for animating the movement of the dots, when to change from HA to A⁻, etc; may have an impact on performance (depending on number of dots, how much they're moving, efficiency of the animation algorithm, etc)
 - User-interface issues: possible confusion or incorrect conclusions when compared to the static presentation in pH Scale sim; controls may be less responsive depending on performance issues
 - None of these issues are particularly difficult, it's just more time (in the ballpark of 4-10 additional hours?). I'll be happy to try it, if that's what you want.
 - o (Kathy) I understand why you want to show motion, but motion seems like it would significantly increase the complexity of the sim, and I am wondering if this is the right sim to try to address that learning goal? I think adding the motion in this panel may draw students attention away from the main connections that we are wanting them to make with this sim. We would NOT worry about collisions, just have the dots do a random walk sort of thing within the liquid as they do in salts and solubility.
 - o (Laurie) I don't think we need to show motion. I'm thinking (like Kathy) that showing the dynamic, close-up process is another sim, and I'm thinking of ways that Salts and Solubility might be a useful template for that.
 - o (Archie) we decided to not include any animation
2. I don't know how important it really is to constantly show the concentration of water.
 - o (Trish) It seems to me that the water concentration doesn't need to appear, but I wasn't sure about higher level applications. I haven't been able to think of a reason for HS or lower grades to use it. In a recent ACS workshop, we were using the concentration of water in order to determine the entropy change for dissolving urea, but that has been the only time we have ever calculated it. The lab is one that I think few HS teachers would attempt, but I used it this year. I have not yet decided if it was worthwhile; I'll be interviewing a few students after break to see if they retained anything from the lab.
 - o (Kathy) I am still thinking that it can be quite useful to have it there, because it reminds students that this is in water, and

- that water is still by far the dominant species. (So not a learning goal that asks them to calculate water concentration ... just much more basic than that.) Does it make the model problematic? I think we could definitely rearrange the *order* of the bars though. (No reason water should be first ... I'm thinking it should be to the far right, as it is in pH scale. And then HA and A⁻ should be to the left - closer to the action.)
- o (Laurie) I do think we should include the H₂O bar; it is the major component of all these solutions. Like Kathy's suggestion about putting it to the right of the graph. So maybe have HA; A⁻; H₃O⁺; OH⁻; H₂O
 - o (Archie) done in version 0.5
3. The graph displays "equilibrium concentrations," not initial concentrations, so we may need to be more specific in our labeling. Or, we might think of how to show "initial concentrations" and/or "equilibrium concentrations."
- o (Kathy) I like the idea of changing the labeling to "equilibrium concentrations". The idea of adding "initial concentrations" is intriguing, but I'd worry about them leaving it set in that mode and then playing with other controls like concentration and strength and not seeing any change in pH, etc. and then just missing the fact that they have it set in initial concentrations?
 - o (Archie) done in version 0.5
4. The pull-down menu should be organized so that "strong acids" is a subheader for all the strong acids, "weak acids" is a subheader for all the weak acids, etc. We don't actually say "strong acid" or "weak acid" anywhere, and this might trigger students to think about comparing various strong acids, various weak acids, and strong versus weak acids, or strong acids versus strong bases. But having the pull-down menu already organized like this gives them some language and makes them wonder, "what do they mean by strong acid or weak acid" and then to explore. ... We'll just use two specific strong bases (NaOH and KOH), so the generic symbol "MOH" won't appear to students.
- o (Archie) decided not to do this, after discussion with Laurie and Kathy. Instead the drop-down will list a generic strong acid and base, a custom weak acid and base, and alphabetically listed real chemicals.
5. It would be helpful to have a lower limit like 0.001 M, instead of zero. Otherwise, how close to zero are we getting? The scale (like all the other scales) will not be linear. Is it a problem to suggest it is by using equal interval tick marks? Perhaps we don't have tick marks? - (Laurie) I'm going to need to do a little research about a few particular acids. For instance, can we even have an 8 M solution of HCN?
- o (Kathy) We can certainly make the concentration slider logarithmic to accommodate the need for that - we need some indication of what the scale represents. Students will have the digital readout so can also see that. So a range of 0.001 to 8, with ticks at 0.001, 0.01, 0.1, and 1. But I think we do want them to be able to go to pure water as comparison, so maybe we just have a "Pure water" in the drop down menu?
 - o (Archie) done in version 0.5
6. Make another tab basically what the current "Solutions" tab is now, with this major suggestion. Maybe we can call it "Comparing Solutions" and there are basically two identical panels that look like the current left-hand panel (with acid / base pull-down menu, concentration slider, and strength slider, and beaker view beneath). So where the bar graph is now, make that another panel with a pull-down menu, concentration slider, and strength slider, with the beaker view beneath. Make the default in both panels "water." Then students can select various acid and base combinations to compare in the two panels. So say a student wants to compare two strong acids. He chooses HNO₃ on the left-hand side and HCl on the right-hand side. Maybe he then chooses to start with the same concentrations of each. He can now compare pH, percent dissociation, etc. of those two solutions. Or perhaps she wants to compare the same acid but at different concentrations. She can set each panel to the same acid and play with concentrations, being able to make direct comparisons in the two panels. Or compare a strong acid with a strong base at the same concentrations.
- o (Archie) "Comparing Solutions" added in version 0.5

Wendy's comments (Dec 30, 2008)

1. I would like to suggest a legend. I realize there is not room in the play area so maybe in a popup window? This might also be good for the pH sim. The only place we define OH⁻ and H₃O⁺ in that sim is via the abstract. I doubt most students even read that. This new sim has even more symbols with no words to attach to. When trying to write this up I found myself switching symbols around and using a where there should be a b. Words might be easier to hold onto until there's meaning for the symbols. Don't know for sure. But if no one is opposed to a legend in a separate window, I think that's a start.
 - o (Chris) Probably best to add a button that displays the legend in it's own window. The alternative would be a menu item, but user's will likely never find it. Also keep in mind that this will result in more text for translators to deal with.
 - o (Kathy) It sounds like you are suggesting that it is like the view reactions button, you can call it up if you need it. That sounds fine to me.
 - o (Laurie) We could have a key, though, that says "HA" = generic weak acid and "A⁻" = what's left when HA dissociates in water. Maybe that would be okay.
 - o (Archie) Legend included in version 0.5.
2. I think something should be different in this notation [HA and A⁻]. I'd suggest H⁺ and OH⁻ or some other symbol that you would not find in the periodic table.
 - o (Kathy) My understanding of the design was that the "A" in HA and A⁻ are going to read the actual compound in all places except for when you select custom acid, in which case it will switch to A to represent the generic acid. "HA" is pretty commonly used
 - o (Wendy) I see now that it's common practice in chemistry to use HA or MOH basically mixing a chemical equation with abbreviations. I'm sure this leads to all sorts of misunderstandings with students. Is there a happy medium where we don't propagate the misconceptions but chemists are still comfortable? I certainly had no idea MOH meant metal hydroxide. I was convinced it was a typo. It's a struggle to get students to understand chemical formulas and I can't imagine how mixing in abbreviations can do anything but muddle this issue. Changing the Font on the abbreviations or something could certainly help with this or even putting in the word metal so you'd have metalOH. I know this makes it

- longer but it's sure more clear. How tied are chemists to using this sort of abbreviation? Is it part of the learning goals that students become familiar with these abbreviations or is this just something that chemistry books do but it's not an important outcome of the sim?
- (Laurie) I'm keeping an eye on Wendy's concerns, and some of them, like using "MOH" shouldn't be an issue. I believe we'll just use two specific strong bases (NaOH and KOH), so the generic symbol "MOH" won't appear to students. In terms of using "HA," "A-," "B" and "BH+" --these will only appear under custom weak acids or custom weak bases. It's the generic symbolism used by chemists, and the words that go with them would be more confusing than just using these symbols, I think. (We could say "weak acid" for "HA" and "conjugate weak base" for "A-" but you see how that will cause confusion since we're not doing conjugate weak acid/weak base pairs in this particular sim.) Wherever we have a specific chemical system, we will use those chemical symbols. We could have a key, though, that says "HA" = generic weak acid and "A-" = what's left when HA dissociates in water. Maybe that would be okay.
 - (Wendy) Is it acceptable to make the A italics or bold or even a different font from the H in HA? That would at least identify this as a different creature from the rest of the symbols. Chris said a legend is possible and I think it'd be a great help in this sim.
 - (Archie) Learning goal concerning A & B symbols included in version 0.5. Symbols "A" "B" and "M" will be italicized.
3. K_a is not defined anywhere in the sim. It appears that the ratio of HCL/CL tells you something about the amount of Hydrogens that disassociated from the Chlorines. The Hydrogens make the Hydronium? But if that was completely true this ratio would just be 1 so some of the hydrogen in the hydroniums have to come from the water and leave some Hydroxide. I may have the science completely wrong (most likely I do) so someone, please straighten me out. I don't want to make too many suggestions until I know the importance of these measurements.
- (Kathy) K_a is $[H_3O^+][A^-]/[HA]$ and represents the products/reactants of the reaction: $HA \rightarrow H_3O^+ + A^-$. This tells you where the equilibrium of the reaction lies -- that is, do you have a lot of products or a lot of reactants. So if you have a lot of products compared to reactants, then the K_a is large and you can conclude that almost all of the HA you add will end up being dissociated (this is strong acid). So by looking at K_a , you can get a sense of how strong your acid is, how much will dissociate (so how much HA you can expect to still find in solution). K_a is not necessarily taught in middle school, so we didn't want it up as default, but for teachers who want to teach to it, this will give students a much better handle on the relationship between the *strength* of an acid and K_a .
 - (Archie) K_a is defined in the "View reaction equations" window (it's been there since Dec 18).
4. I have no theory at all as to why the label is "Custom Weak Acid" rather than "Custom Acid" and similarly there is "Custom Weak base" and not just Custom Base. I assume there's some limit with what the sim can demonstrate??
- (Kathy) Laurie and Trish both felt it was quite problematic having a continuum between weak and strong, so this is what we came up with that they felt comfortable with. Perhaps they can elaborate more on the troubles with just one continuum.
5. I don't know why Strong Acid is (HA), Custom Weak Acid is also (HA), Strong Base is (MOH) and Custom Weak Base is (B). Really no guess at all.
- (Kathy) Many strong acids have the same structure as weak acids (an HA). But most strong bases are a metal hydroxide (MOH) where as weak bases have a different structure (B) which then grabs a proton to make (BH). It is the OH in the MOH that comes off and makes it basic. I think if the sim was working and you saw that KOH and NaOH were all strong bases, you might have started to make sense of why MOH was used for a strong base with M representing K or Na.
6. I'm also confused by showing Hydrochloric Acid versus Chlorine. How is this related or different from showing Hydronium and Hydroxide ratio? I vaguely remember this being a misconception? Students think pH tells you the strength of the acid but actually is a measure of how acidic or basic something is and the strength of the acid is more like concentration. But that can't be quite right since you have both an acid strength and acid concentration slider. From reading the learning goals I'm thinking the Acid or Base causes the water to dissociate into Hydronium and Hydroxide? That is the pH?? Many of these questions would be answered if I could play with the sim and see what happens to all these ratios. I'd like to be able to add Acid to water and watch what happens but that's titration right?
- (Kathy) Looking at the A-/HA ratio tells you the strength of the acid (how much of it has dissociated). If you have a very small amount of acid, then the pH can still be close to neutral even if you have a strong acid. So as you increase the concentration, you will then see the H_3O^+/OH^- ratio change and the pH change, even though you have the same acid (strong) and the A-/HA ratio isn't really changing (almost all A-). You are adding acid to water here, that is the concentration. The higher the concentration the higher the acid to water ratio. But this concentration is the amount of acid before it was added to the water (so that is the HA + A-). This is a subtle issue that is often not addressed in chemistry courses, but which you can teach to using the sim. Titration is when you have water, add some acid to make it acidic, and then titrate with some base to bring it back to neutral.

Will the symbols need to be translatable? (Jan 2009) (Answer: No)

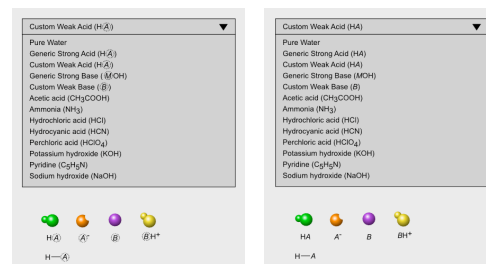
- (Marj) Looks like we're fine. I've heard from Vietnamese, Russian, and Arabic. I think I may need to look for Chinese contacts that aren't translators to get a specific answer for that language.
- (Marj to Jia Shi of the CU-SEI) Could you let me know how chemical formulas are written in Chinese? Are they written as we write them in English, for instance water as H₂O? We're developing a new PhET sim and are trying to figure out if the chemical formulas will need to be translatable.
 - (Jia) I think this is not a concern. Chemical formulas are written in China as we write them, i.e. CO₂ and H₂O etc. Of course Chinese characters will be written under each formula as well.
- (Wendy) I just heard from the Hewlett Chinese translator and they use HCL so don't need to translate it!
 - (Chris) Not sure how to interpret this piece of news... Is this one more data point, or is it a decision that we don't need to translate chemical formulae?
 - (Wendy) It's a decision to not translate chemical formulas.
- (Archie) It appears that the symbol " K_a " should actually have a subscripted "a". Will this make for problems if people need to

translate " K_a " into something else in another language?

- (Chris) Subscripts and superscripts are implemented using HTML. In this case, the string would be "<html>K_a</html>". This makes translation more difficult for the translator, because he/she must know HTML syntax. But we require this in many other places, so it's nothing new.

generic acid-base symbols "A", "B" and "M" (Jan 13 2009)

- (Archie) Kathy, Wendy, Noah and I talked today about a new way to help students with the "generic" acid and base symbols that we use in the sim. We now use "HA" for a generic acid and "B" for a generic base. We would like to try to distinguish these symbols from standard atomic symbols. The Olmsted and Williams Chemistry textbook appears to do this by italicizing the A or B. We also talked about using an additional mark such as a circle around the letter. I mocked up these two approaches, as they would appear in the drop-down menu, the bar chart labels, and a simple Lewis structure. (Chris says that graphics in the drop-down are not a problem.) Please take a look at the two images at the right (click them for larger images). I'd like to hear what you think of them, or if you have some other ideas for making these symbols less confusing to those who are not fluent in the chemistry lingo.
- (Wendy) I really like the dotted line version. It is hard to notice a difference with the italics version.
- (Laurie) I'm okay with italicizing the "A" and the "B." I'm concerned that putting a circle around them conveys that they are single atoms, when they really just represent "the rest of the molecule."
- (Chris) The version that shows text with some italics is pretty easy, just use HTML to do the italics. Having to deal with HTML will some complication for the translators. The version with the dotted-circle-around-letters... no idea how I could do that. I guess the circled letters could be images, but there's no way I could make them flow so seamlessly with the text. Font sizes vary by platform, so plan on the text and image fonts not matching. And Java labels only provide the ability to put an icon next to text (not on top of text, or in the middle of text). If this is what Archie was asking me about, then I must retract my "not a problem" prognosis.
 - (Archie) I think the entire chemical symbol, circle and letters and all, would be a graphic (if we went that way). We've already determined that they do not need to be translatable.
- (Kathy) How about we try italics and then see what interviews show?
- (Archie) Ok, we're going with italics only for now (version 0.5).



range of K_a for custom weak acids (Jan 14 2009)

- (Kathy) [Wikipedia says](#) that K_a values below 100 signify "weak acids". So to see the greatest amount of change in the various quantities for our custom weak acid, we should use a range of K_a that goes all the way up to 100.

List of common acids and bases

Acids:

HCl	Hydrochloric acid	Ka = Strong $\text{HCl (aq)} + \text{H}_2\text{O (l)} \rightarrow \text{H}_3\text{O}^+ \text{ (aq)} + \text{Cl}^- \text{ (aq)}$
HClO_4	Perchloric acid	Ka = Strong $\text{HClO}_4 \text{ (aq)} + \text{H}_2\text{O (l)} \rightarrow \text{H}_3\text{O}^+ \text{ (aq)} + \text{ClO}_4^- \text{ (aq)}$
HClO_2	Chlorous acid	Ka = 1×10^{-2} $\text{HClO}_2 \text{ (aq)} + \text{H}_2\text{O (l)} \leftrightarrow \text{H}_3\text{O}^+ \text{ (aq)} + \text{ClO}_2^- \text{ (aq)}$
HClO	Hypochlorous acid	Ka = 2.9×10^{-8} $\text{HClO (aq)} + \text{H}_2\text{O (l)} \leftrightarrow \text{H}_3\text{O}^+ \text{ (aq)} + \text{ClO}^- \text{ (aq)}$
HBrO	Hypobromous acid	Ka = 2.3×10^{-9} $\text{HBrO (aq)} + \text{H}_2\text{O (l)} \leftrightarrow \text{H}_3\text{O}^+ \text{ (aq)} + \text{BrO}^- \text{ (aq)}$
HNO_3	Nitric acid	Ka = Strong $\text{HNO}_3 \text{ (aq)} + \text{H}_2\text{O (l)} \rightarrow \text{H}_3\text{O}^+ \text{ (aq)} + \text{NO}_3^- \text{ (aq)}$

HNO ₂	Nitrous acid	K _a = 7.2 × 10 ⁻⁴ HNO ₂ (aq) + H ₂ O (l) ↔ H ₃ O ⁺ (aq) + NO ₂ ⁻ (aq)
HF	Hydrofluoric acid	K _a = 6.8 × 10 ⁻⁴ HF (aq) + H ₂ O (l) ↔ H ₃ O ⁺ (aq) + F ⁻ (aq)
HCOOH	Formic acid (found in ants)	K _a = 1.7 × 10 ⁻⁴ HCOOH (aq) + H ₂ O (l) ↔ H ₃ O ⁺ (aq) + HCOO ⁻ (aq)
CH ₃ COOH	Acetic acid (found in vinegar)	K _a = 1.8 × 10 ⁻⁵ CH ₃ COOH (aq) + H ₂ O (l) ↔ H ₃ O ⁺ (aq) + CH ₃ COO ⁻ (aq)
CH ₃ CH(OH)COOH	Lactic acid (found in milk)	K _a = 1.4 × 10 ⁻⁴ CH ₃ CH(OH)COOH (aq) + H ₂ O (l) ↔ H ₃ O ⁺ (aq) + CH ₃ CH(OH)COO ⁻ (aq)
HCN	Hydrocyanic acid	K _a = 6.2 × 10 ⁻¹⁰ HCN (aq) + H ₂ O (l) ↔ H ₃ O ⁺ (aq) + CN ⁻ (aq)

Bases:

NaOH	Sodium hydroxide	K _b = Strong NaOH (aq) → Na ⁺ (aq) + OH ⁻ (aq)
KOH	Potassium hydroxide	K _b = Strong KOH (aq) → K ⁺ (aq) + OH ⁻ (aq)
NH ₃	Ammonia (found in window cleaner)	K _b = 1.8 × 10 ⁻⁵ NH ₃ (aq) + H ₂ O(l) ↔ NH ₄ ⁺ (aq) + OH ⁻ (aq)
CH ₃ NH ₂	Methylamine	K _b = 4.4 × 10 ⁻⁴ CH ₃ NH ₂ (aq) + H ₂ O(l) ↔ CH ₃ NH ₃ ⁺ (aq) + OH ⁻ (aq)
C ₅ H ₅ N	Pyridine	K _b = 1.7 × 10 ⁻⁹ C ₅ H ₅ N(aq) + H ₂ O(l) ↔ C ₅ H ₅ NH ⁺ (aq) + OH ⁻ (aq)