Web App Port of Buffer Capacity Matlab Application

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Context

- pH = "potential of Hydrogen"
  - acidity/basicity of substance
  - $pH = -\log([H^+])$, ($[H^+]$ is the hydrogen ion concentration)
- pH > 4.6 in sealed container = home for clostridium botulinum
  - Clostridium botulinum create toxin that causes botulism
  - Botulism = Fatal disease

How to combat botulism?

- Make foods more acidic
  - pH < 4.6
  - $[H^+] > 10^{-4.6}$
- We don't know $[H^+]$
- But we know how to find it

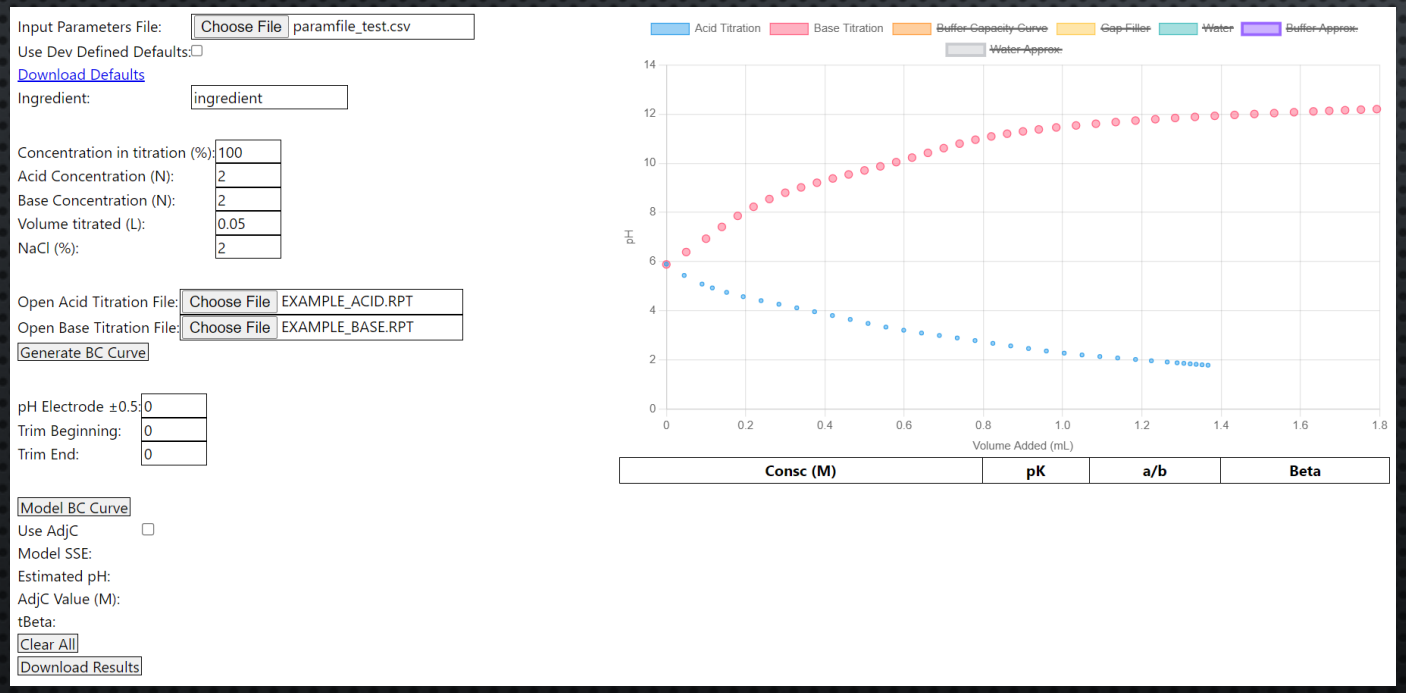
How to find $[H^+]$

- $0 = \sum \frac{C_{ai} K_{ai}}{K_{ai} + [H^+]} - \sum \frac{C_{bi} [H^+]}{K_{bi} + [H^+]} + \frac{K_w}{[H^+]} - [H^+] + AdjC$
- $C_{a/b}$: Vector of the molar concentrations of acids and bases
- $K_{a/b}$: Vector of corresponding equilibrium constants of acids and bases
- $K_w = 1 \times 10^{-14}$: autoionization constant of water
- $AdjC$: Ion contribution due to salt in acid and bases
- Better Idea! Machine learning
  - Newton minimization

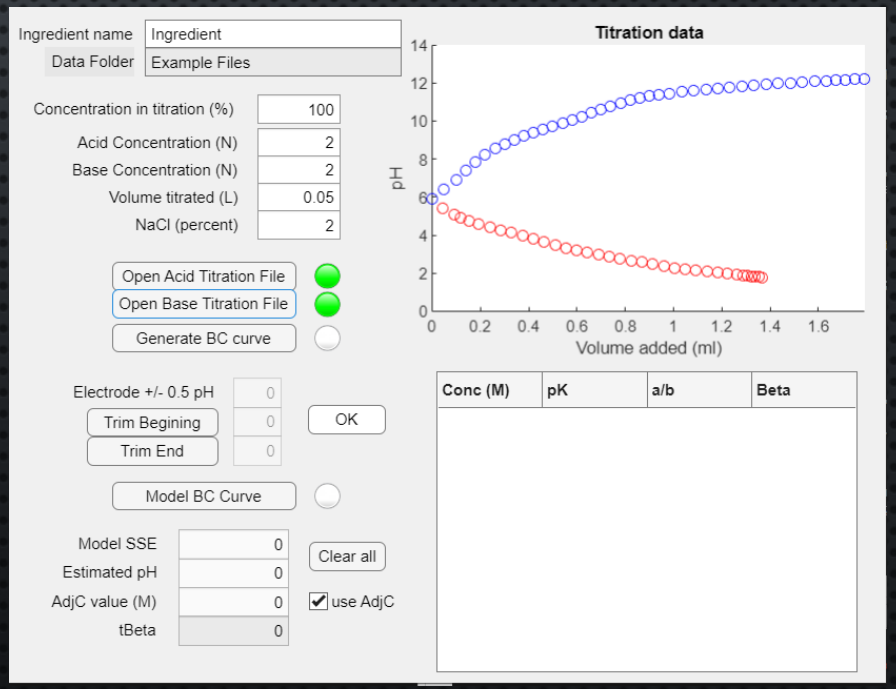
VISUAL COMPARISON

Accept parameters (.csv file)
Accept titration data from Hanna Instruments automated titrator (.RPT files)

BufferSDWebApp



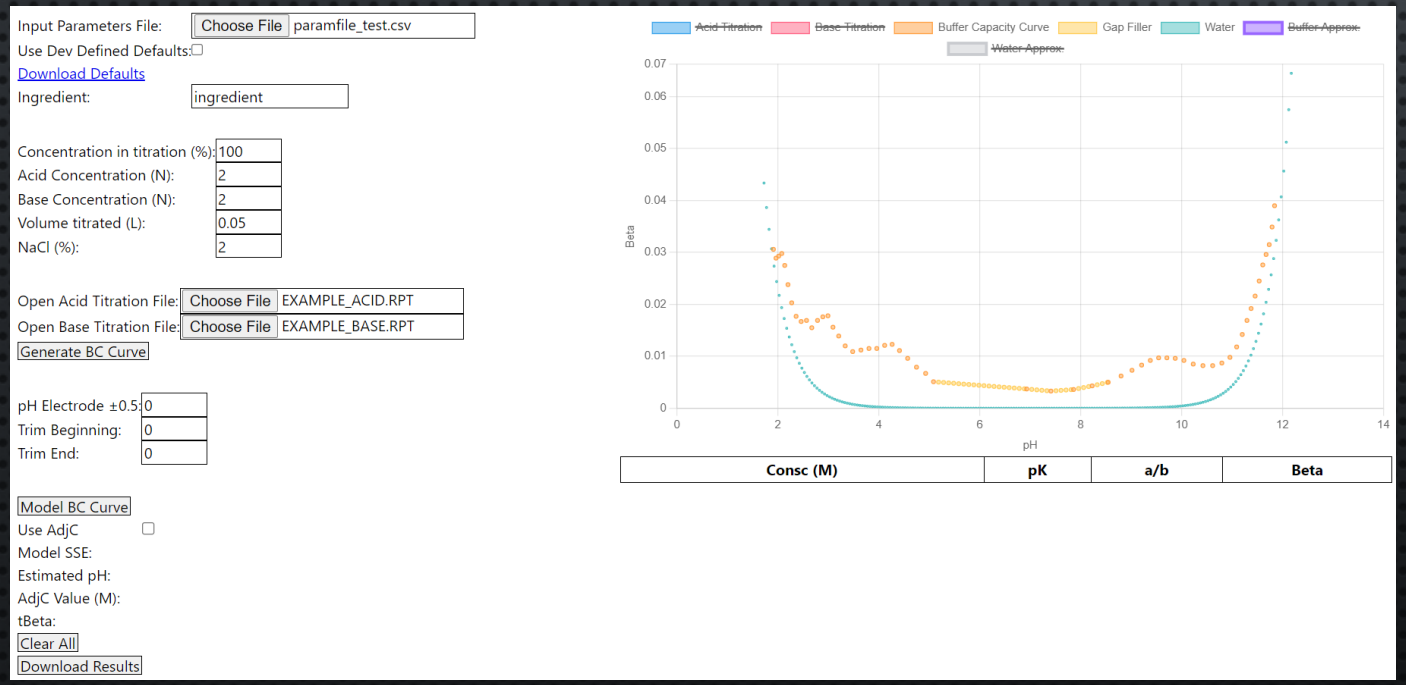
BufferCapacity3



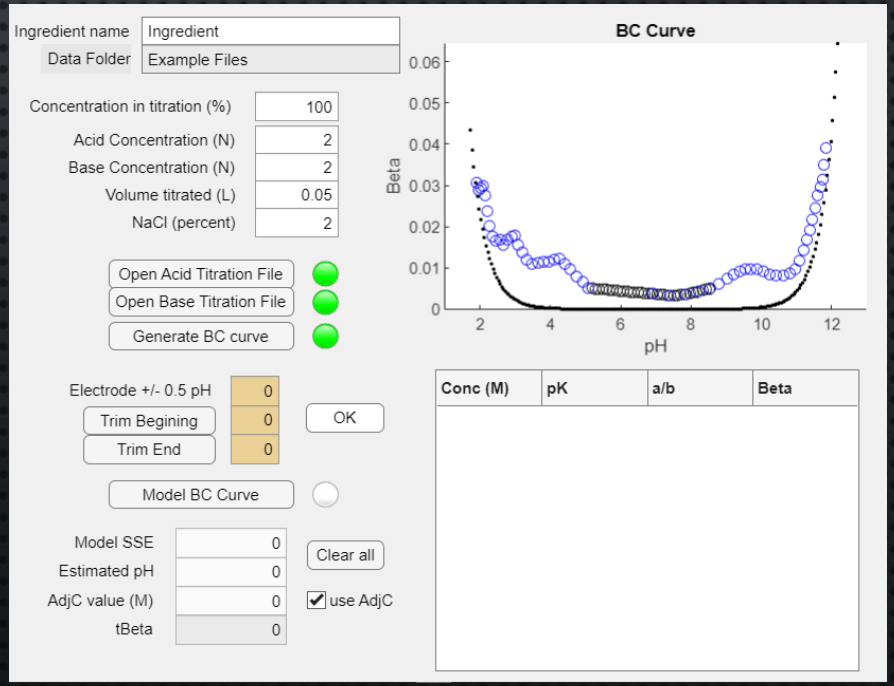
VISUAL COMPARISON

Generate buffer capacity curve via $\beta = \frac{\Delta(\text{acid or base})}{\Delta pH}$

BufferSDWebApp



BufferCapacity3



VISUAL COMPARISON

$$\min_{x} \sum_{i=1}^{n} \left(Y(pH_i) - F(pH_i; \boldsymbol{x})\right)^2$$

$Y(y)$ = observed buffer capacity at pH y

$$F(y; \boldsymbol{x}) = B_0 + \sum A_i \sin(\frac{i}{2} y) + \sum B_i \cos(\frac{i}{2} y), (A_i, B_i \epsilon \boldsymbol{x})$$

$$\beta([H^+]; \boldsymbol{x}) = 2.3 \sum_i^n \frac{C_i K_i [H^+]}{(K_i + [H^+])^2} + \frac{K_w}{[H^+]} + [H^+]$$ predicted buffer capacity at $[H^+]$ given $\boldsymbol{x}$

BufferSDWebApp

Input Parameters File: Choose File paramfile_test.csv

Use Dev Defined Defaults:

Download Defaults

Ingredient: ingredient

Concentration in titration (%): 100

Acid Concentration (N): 2

Base Concentration (N): 2

Volume titrated (L): 0.05

NaCl (%): 2

Open Acid Titration File: Choose File EXAMPLE_ACID.RPT

Open Base Titration File: Choose File EXAMPLE_BASE.RPT

Generate BC Curve

pH Electrode ±0.5: 0

Trim Beginning: 0

Trim End: 0

Model BC Curve

Use AdjC

Model SSE: 5.847e-5

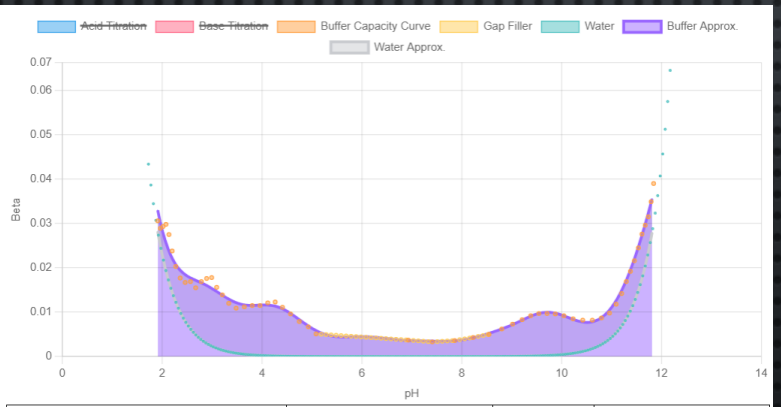
Estimated pH: 5.891

AdjC Value (M): 0.02169

tBeta: 7.251

Clear All

Download Results



Consc (M)	pK	a/b	Beta
0.0203	2.8179	a	0.0152
0.0164	4.2775	a	0.0096
0.0059	6.0909	a	0.0034
0.0037	7.3143	b	0.0021
0.0047	8.6075	b	0.0027
0.0150	9.7302	b	0.0088
0.0370	12.0000	b	0.0443

BufferCapacity3

Ingredient name: Ingredient

Data Folder: Example Files

Concentration in titration (%): 100

Acid Concentration (N): 2

Base Concentration (N): 2

Volume titrated (L): 0.05

NaCl (percent): 2

Open Acid Titration File

Open Base Titration File

Generate BC curve

Electrode +/- 0.5 pH: 0

Trim Begining: 0

Trim End: 0

OK

Model BC Curve

Model SSE: 5.848e-05

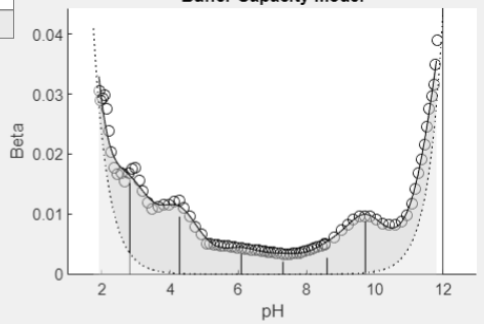
Estimated pH: 5.889

AdjC value (M): 0.02169

tBeta: 7.252

Clear all

use AdjC



Conc (M)	pK	a/b	Beta
0.0203	2.8179	a	0.0152
0.0164	4.2774	a	0.0096
0.0059	6.0908	a	0.0034
0.0037	7.3143	b	0.0021
0.0047	8.6077	b	0.0027
0.0150	9.7302	b	0.0088
0.0370	11.9998	b	0.0443

DETAIL COMPARISON

BufferCapacity3	BufferSDWebApp
MATLAB	Python, HTML, CSS, JavaScript
Desktop Application (>1GB)	Web Application (long load time)
fmincon	*scipy.optimize.minimize* method = "trust-constr"
fminsearch	*scipy.optimize.minimize* method = "Nelder-Mead"
MATLAB App Designer	Flask

DATA COMPARISONS

Ingredient (Program)	Anchovy MS1 (BC3)	Anchovy MS1 (BSD)	Avocado MS4 (BC3)	Avocado MS4 (BSD)	Buttermilk MS15 (BC3)	Buttermilk MS15 (BSD)
SSE	2.18E-04	2.17E-04	6.96E-05	6.96E-05	9.48E-06	3.72E-05
Estimated pH	5.848	5.843	5.335	5.350	6.676	6.676
AdjC	-0.053	-0.053	-0.022	-0.022	-0.021	-0.022
tBeta	11.398	11.370	4.199	4.199	5.333	6.027

$$MRD = \frac{1}{3}\sum_{i=1}^{3}\frac{|BC3_i - BSD_i|}{BC3_i}$$

SSE	Estimated pH	AdjC	tBeta
0.9762	0.0012	0.0159	0.0442

CLIENT-SIDE ONLY

- COMPANIES DON'T WANT TO SHARE THEIR RECIPES
- COMPANIES DON'T WANT TO SEND THEIR RECIPES TO OTHER SERVERS
- SOLUTION: DON'T MAKE THEM SEND IT TO A SERVER
  - PYSCRIPT: INTERNAL ANACONDA PROJECT
  - ALLOWS PYTHON TO RUN CLIENT-SIDE

INGREDIENTS: ENRICHED FLOUR (WHEAT FLOUR, NIACIN, REDUCED IRON, THIAMIN MONONITRATE [VITAMIN B_1], RIBOFLAVIN [VITAMIN B_2], FOLIC ACID), CORN SYRUP, SUGAR, SOYBEAN AND PALM OIL (WITH TBHQ FOR FRESHNESS), CORN SYRUP SOLIDS, DEXTROSE, HIGH FRUCTOSE CORN SYRUP, FRUCTOSE, GLYCERIN, CONTAINS 2% OR LESS OF COCOA (PROCESSED WITH ALKALI), POLYDEXTROSE, MODIFIED CORN STARCH, SALT, DRIED CREAM, CALCIUM CARBONATE, CORNSTARCH, LEAVENING (BAKING SODA, SODIUM ACID PYROPHOSPHATE, MONOCALCIUM PHOSPHATE, CALCIUM SULFATE), DISTILLED MONOGLYCERIDES, HYDROGENATED PALM KERNEL OIL, SODIUM STEAROYL LACTYLATE, GELATIN, COLOR ADDED, SOY LECITHIN, DATEM, NATURAL AND ARTIFICIAL FLAVOR, VANILLA EXTRACT, CARNAUBA WAX, XANTHAN GUM, VITAMIN A PALMITATE, YELLOW #5 LAKE, RED #40 LAKE, CARAMEL COLOR, NIACINAMIDE, BLUE #2 LAKE, REDUCED IRON, YELLOW #6 LAKE, PYRIDOXINE HYDROCHLORIDE (VITAMIN B_6), RIBOFLAVIN (VITAMIN B_2), THIAMIN HYDROCHLORIDE (VITAMIN B_1), CITRIC ACID, FOLIC ACID, RED #40, YELLOW #5, YELLOW #6, BLUE #2, BLUE #1.

Without Pyscript

Interpreter for Javascript and WebAssembly

Interpreter for Python, Java, R, etc.

Python:
C = (A+B)^2

Assembly:
MOV AX, [A] ; Move A to Register Ax
ADD AX, [B] ; Add B to A
IMUL AX ; Square(A+B)
MOV [C], AX ; Mov (A+B)^2 to C

Machine Code:
00000100 A10D01
00000103 03060F01
00000107 F7E8
00000109 A31101
0000010C C3
0000010D 0300
0000010F 0400
00000111 0000

Thank you StackOverflow!

Without Pyscript

Interpreter for Javascript and WebAssembly

Interpreter for Python, Java, R, etc.

With Pyscript

Pyodide translates functions to bytecode

SECURITY

What comes next?

- Deployment on publicly available server
- Use it to produce pH estimations for multiple ingredients