

Integrating the iPhone and iPad with Mass & Energy Balances



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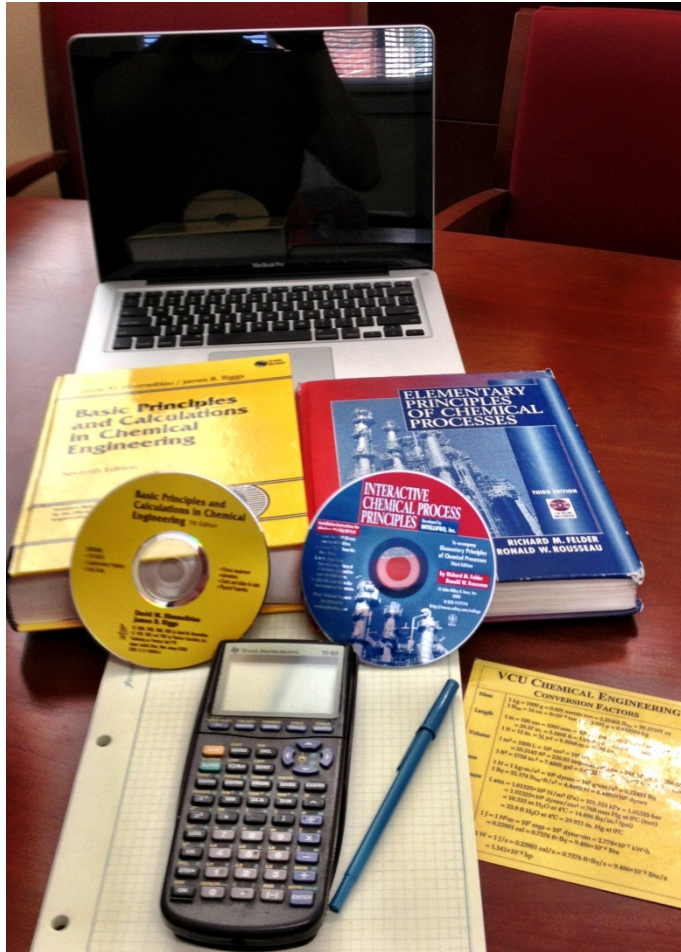
AIChE Annual Meeting – Pittsburgh, PA
October 29, 2012

Collaborators

- John Patrick “JP” McLemore
 - Co-creator of ChemE App, UA ChBE Grad BS, MS 2012
 - Currently with Schlumberger (Aberdeen, Scotland)
- Prof. Heath Turner – UA ChBE
- David Roveda
 - UA ChBE undergrad
- University of Alabama Computer Based Honors (CBH) Program



A Crossroads in How We Work & Teach



The bare essentials...

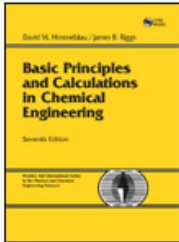


*“The Bara Essentials”...
Can we do more with less?*

An Example “App” from the Year 2000

Basic Principles and Calculations in Chemical Engineering, 7th Edition

[about](#) | [requirements](#) | [tech support](#)



David M. Himmelblau and James B. Riggs
ISBN: 0131406345
Published November 2003
Prentice Hall PTR
One Lake Street, Upper Saddle River, NJ, 07458
Online at <http://www.phptr.com/>

About the CD

This CD contains text and supplementary material associated with the book.

Please note that you will need Adobe Acrobat Reader and a web browser to use the CD.

CD Contents

This CD includes the following resources:

Software

- [Polymath](#)—solves linear and nonlinear algebraic equations
- [PhysProp](#)—software used to retrieve critical properties

Problem Solving

- [Workbook](#)—100 problems solved in detail plus 100 more
- [Problem Solving](#)—suggestions on how to improve problem solving

Charts

- [Compressibility Charts](#)—compressibility charts for various gases
- [Psychrometric Charts](#)—two psychrometric charts for air-water vapor mixtures

Process Equipment

Chemical Engineering

Physical Properties | Heat Capacities | Enthalpies | Density of Liquid | Vapor Pressure | Steam Tables

Compounds

Miscellaneous

AMMONIA

A - D

1,1-DICHLOROETHANE

E - H

1-EICOSANETHIOL

I - L

1-IODOPROPANE

M - Q

1,2-PENTADIENE

R - X

1,1,1-TRIFLUOROETHANE

Formula

AR
BR2
CL2
CS2
F2
H2
...

CCL4
CCL3F
CCL2F2
CCLF3
CF4
CO
...

AMMONIA

Formula H3N

Molecular weight (g mol) 17.031

Freezing Point (K) 195.4

Boiling Point (K) 239.7

Critical Temperature (K) 405.6

Critical Pressure (bar) 112.7469

Critical Volume (cm³/mol) 72.5

Critical Density (g/cm³) 0.235

Critical Compressibility (Z_c) 0.242

Ascentric Factor (ω) 0.25

Enthalpy of Formation (kJ/g mol) -45.68928(g)
(at 298.15K)

Enthalpy of Vaporization (kJ/g mol) 23.251
(at normal boiling point)

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David
Himmelblau



Motivation behind the ChemE App

- Began teaching Mass & Energy Balances in Sp. 2011
 - Started using iPod Touch in 2010
- Lack of truly functional ChemE apps
 - Few selections/poor functionality
- Quickly found that solving equations by hand takes time away from instruction
 - Look up values/constants in table, input into calculator or Excel
- Want to rapidly (i.e. instantaneously) graph data
- **Goal: Integrate a deep set of thermophysical properties with problem solving tools and data sharing capabilities**
 - *And make it visually attractive!*





Why iOS (Apple) Hardware?



- Survey of Mass & Energy Balance class showed strong student preference for Apple products
- Of those owning smartphones (31/43), 80% owned iPhones, with another 7/43 planning to buy an iPhone.
 - Potentially 90% of class will be on iOS platform in near future
 - Only 10% of class using Android phones
 - ~25% of class already own an iPad with another 25% planning to buy an iPad.

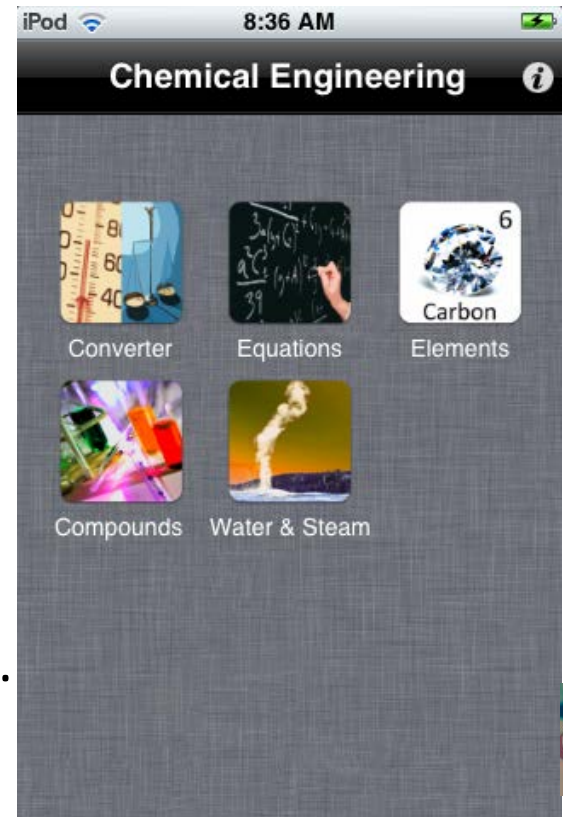
Coding & Distribution for iOS Devices

- Programming in Objective-C via the Xcode interface
 - Only available on Apple desktops and laptops
- Requires both traditional code writing and design of visual interfaces
- Code and interfaces must be reviewed and approved by Apple prior to release on App Store
 - Strict quality requirements
 - 7-10 day wait before new versions are available
- Apple provides software direct to user
 - Software owner decides price (our apps are free!)
 - Developers pay \$99/year fee



Chemical Engineering App

- Chemical Engineering App – January 2012
 - Formatted for iPhone & iPod Touch, usable on iPad
 - >2700 downloads to date
- Features
 - Properties for 1000+ compounds and elements
 - Plus links to external sources with additional info
 - Converters for a variety of units
 - Steam tables
 - Equations of State
 - Ideal gas, RK, vdW, SRK, Lee-Kesler comp.
 - Antoine Equation, Heat Capacity, Pressure Head



iPhone Screenshots

iPod 8:36 AM

Compound

acetone
Compound

2-propanone
Common Names

C₃H₆O
Formula

67-64-1
CAS Number

[View in Wikipedia](#)

iPod 4:31 PM

58.08
Molecular Weight

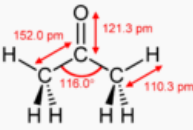
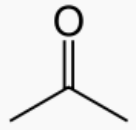
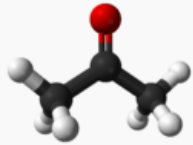
0.791
Density (g/mL)

-95
Melting Temperature (Celsi)

5.69
Heat of Fusion (kJ/mol)

Acetone

Acetone^[1]


IUPAC name
2-Propanone

Systematic name
Propan-2-one^[2]

Other names
Dimethyl ketone^[3]

iPod 8:37 AM

Pressure

atm: 0.59868

bar: 0.60662

psi: 8.7982

mmHg: 455

iPod 8:36 AM

Saturated Steam

Temp: °C

Pressure: bar

Liquid Cp: 4.184 kJ/kg-K

Vapor Cp: 1.957 kJ/kg-K

Liquid Cv: 3.997 kJ/kg-K

Vapor Cv: 1.474 kJ/kg-K

Liquid Density: 985.2 kg/m³

Vapor Density: 0.1094 kg/m³

Liquid Enthalpy: 234.4 kJ/kg

iPod 8:36 AM

Antoine Calc

1,1-difluoroethane

T: **34** Celsius

P: **5709.8** mmHg

A: 7.03

B: 910

C: 244

Lower Temperature Limit in Celsius: -35

Upper Temperature Limit in Celsius: 0

Chemical Engineering AppSuite HD

- Chemical Engineering App – May 2012

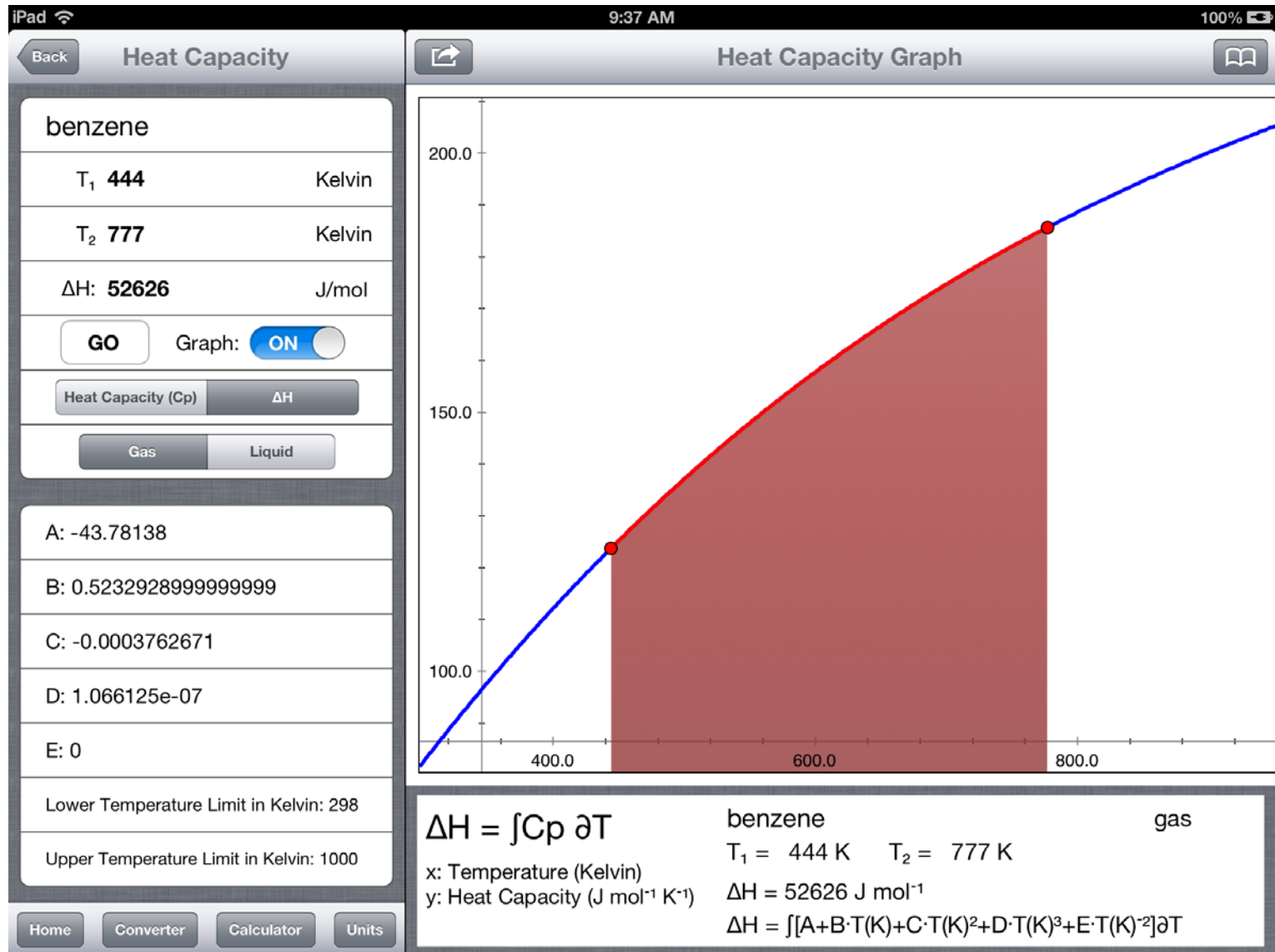
- Exclusive to iPad
- >3500 downloads to date

- Features

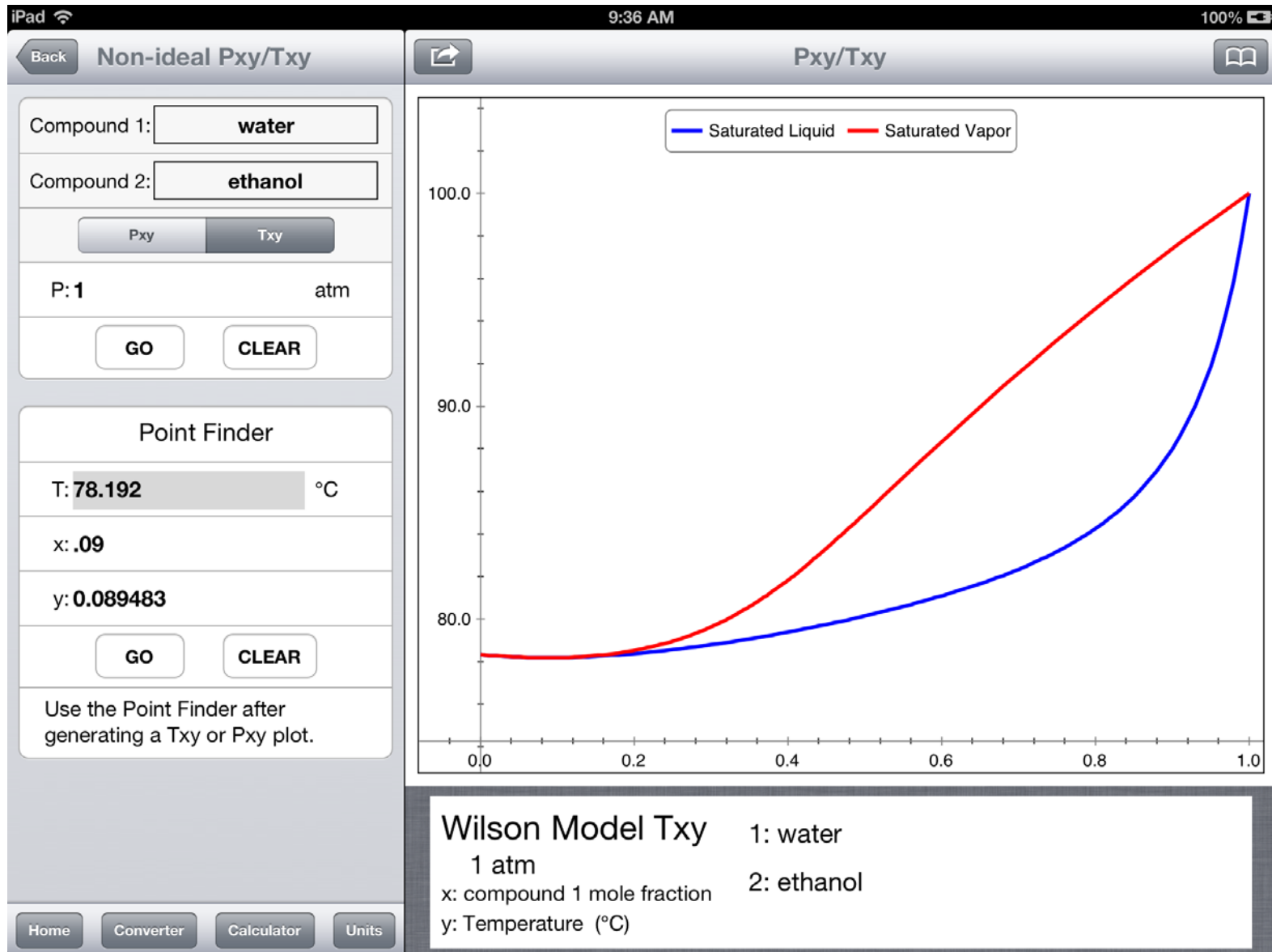
- All of iPhone functions
- **Graphing**
- VLE calculation
- Newtonian Fluids
- Matrix Operations
- Spreadsheets, Calculator
- “ChemE Tools”
- Ability to save work
- Reference data as PDFs
- Integration with Twitter and email



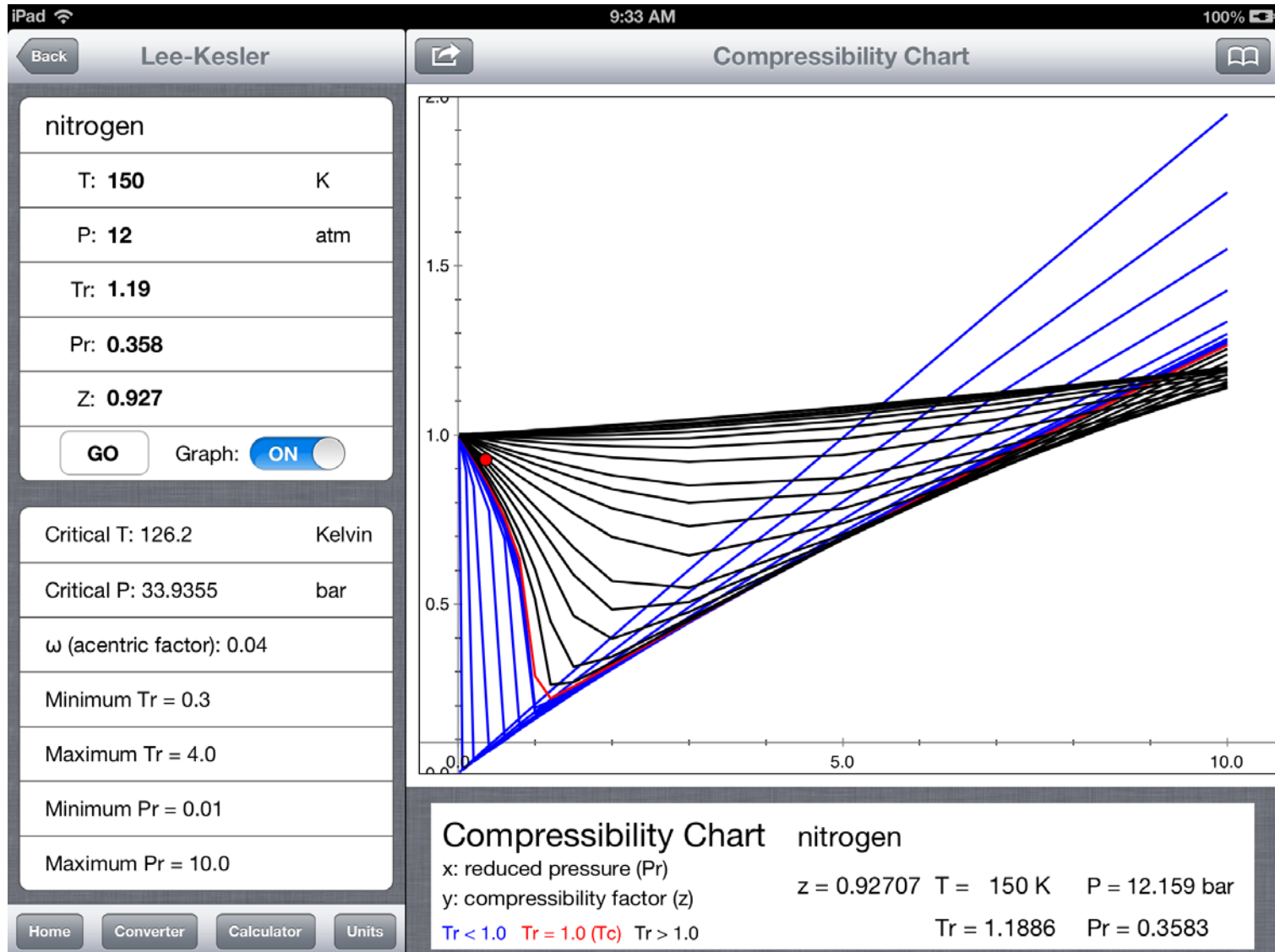
iPad – Heat Capacity & ΔH



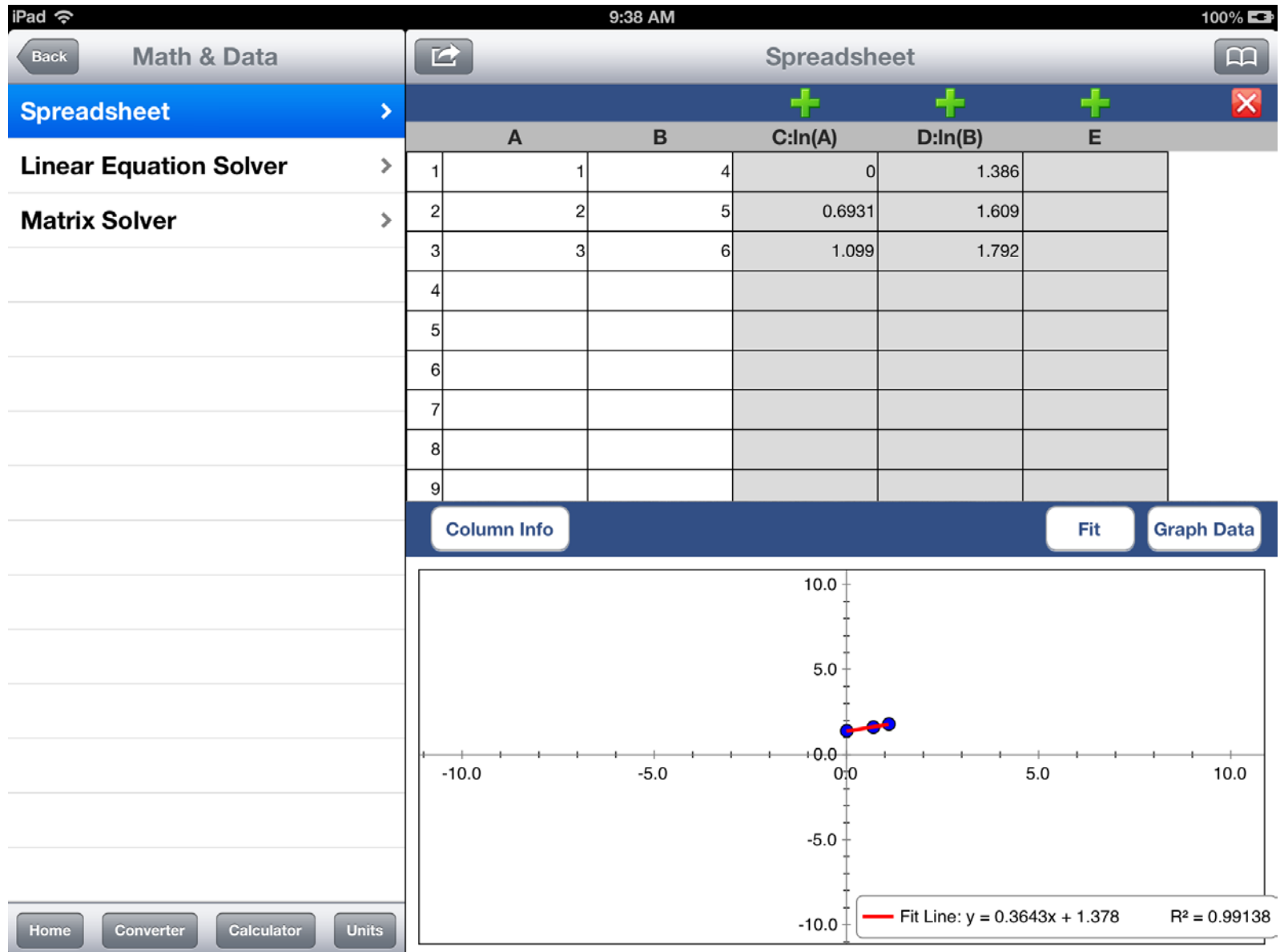
iPad – VLE Txy Diagram



iPad – Lee-Kesler Compressibility



iPad – Spreadsheet w/ Graphing



iPad – Linear Equation Solver

iPad 9:40 AM 100%

Back Math & Data

Linear Equation Solver

Equations: 3 Variables: x_1, x_2, x_3 Add Equation

Spreadsheet >

Linear Equation Solver > $x_1 + x_2 + x_3 - 5 = 0$

Matrix Solver > $x_1 - 2x_2 - 3x_3 + 4 = 0$

$x_1 - 3x_2 + 4x_3 - 5 = 0$

Solvable: YES Clear All

Input Matrix:

$[x_1, x_2, x_3, \text{Remainder}]$
$[1, 1, 1, 5]$
$[1, -2, -3, -4]$
$[1, -3, 4, 5]$

Solution:

$x_1 = 2.48$
 $x_2 = 1.08$
 $x_3 = 1.44$

Solution Check:

$x_1 + x_2 + x_3 - 5 = 0$
 $x_1 - 2x_2 - 3x_3 + 4 = 0$
 $x_1 - 3x_2 + 4x_3 - 5 = 0$

Home Converter Calculator Units

Student Response

- Students have been overwhelmingly enthusiastic about using their iPhones and iPad to solve problems in class
 - iPhone includes a calculator... iPad does not
 - Most had not considered these devices in this light
 - View technology primarily for entertainment/communications purposes(Facebook, Twitter, YouTube, Instagram, Reddit, etc.)



- Appreciate accessibility of spreadsheet, matrix tools
 - Students can be intimidated by Excel, Matlab

Challenges

- Not all students have iPhones & iPads
 - Can we require an iPad as part of the ChemE curriculum?
 - Some cite cost as a barrier (\$500+), but new iPad mini may lower the activation energy (\$350)
- How user-friendly should the software be?
 - Do we allow students to make mistakes and input “bad” values (i.e. mass fraction > 1)
- Great for well-defined equations but can we make it more open-ended?
 - i.e. interactively design and solve flowcharts?

Teaching Benefits

- This software saves time!
 - Not spending time solving equations by hand or looking in data table during class
 - iPad can be shown on projector
 - I am a week ahead of last semester's pace
- Students are excited by the visuals
 - See the behavior of functions vs. temp, shapes of molecules, build graphs rapidly
 - Appeal to different learning styles
- Enhance content in mass & energy balances
 - Pull in concepts from thermodynamics
 - e.g. rapidly compare ideal gas law to other EOS

Current & Near Future Plans

- Build the base
 - App exposure is still very limited
 - Actively communicate with and get feedback from users



- Implement interactive practice problems
 - Code written to generate highly randomized mass balance questions
 - First examples will be live on iPad by end of 2012
- More tools, more data, more integration!



Thank You!

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