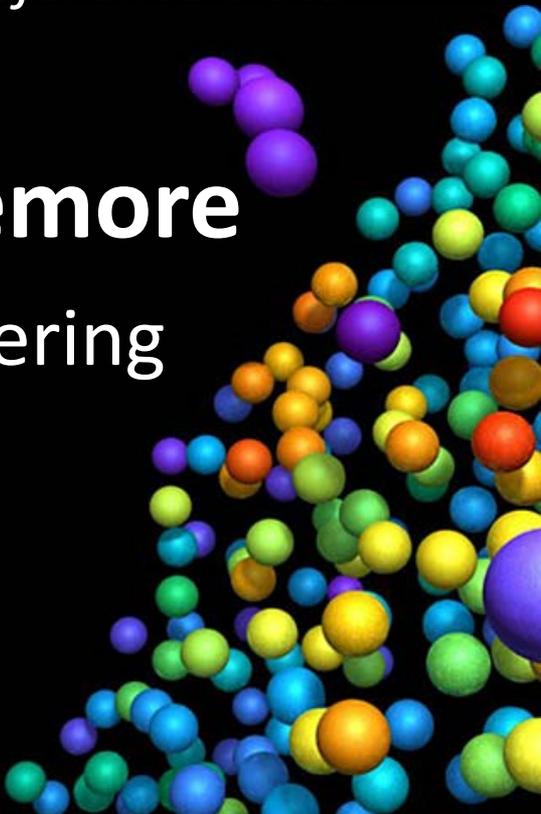


Chemical Engineering App:

*Increasing Accessibility of Course Materials, Reference Data
and Problem Solving Tools*

Jason E. Bara & J.P. McLemore

Chemical & Biological Engineering
University of Alabama



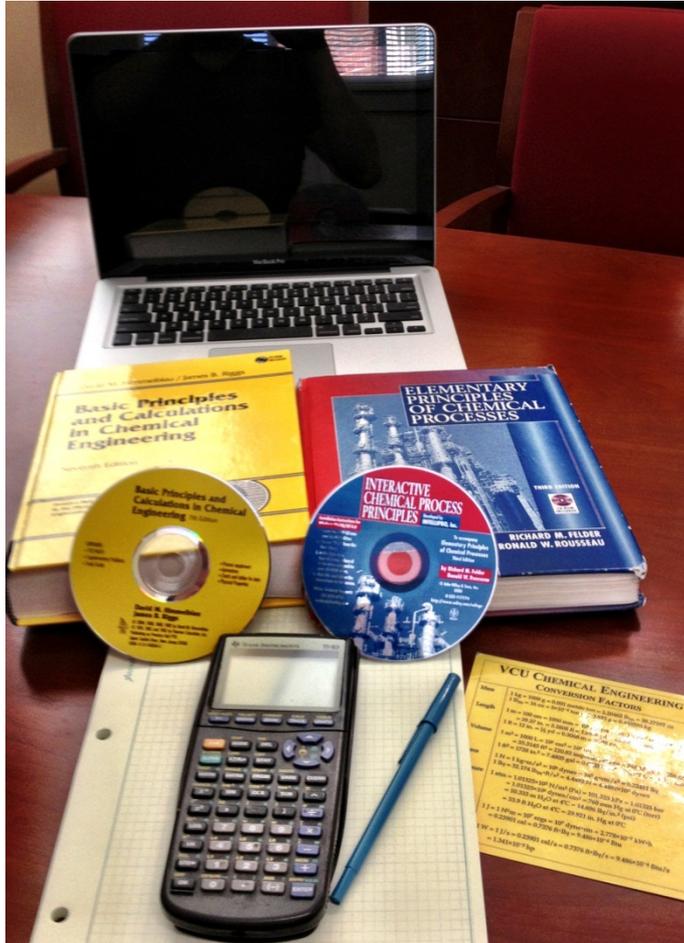
AIChE Annual Meeting
San Francisco, CA
November 6, 2013

Collaborators

- John Patrick “JP” McLemore – MS 2012
 - Currently with Schlumberger (Aberdeen, Scotland)
- Prof. Heath Turner – UA ChBE
- David Roveda
 - UA ChBE undergrad
- Anna Marthinsen
 - UA CS undergrad
- University of Alabama Computer Based Honors (CBH) Program



A Crossroads in How We Work & Teach



The bare essentials...

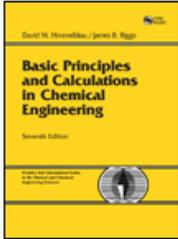


Can we do more with less?

An "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 CD-ROM drive to use this CD.

CD Contents

This CD includes the following resources:

Software

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

Problem Solving

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

Charts

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

Process Equipment

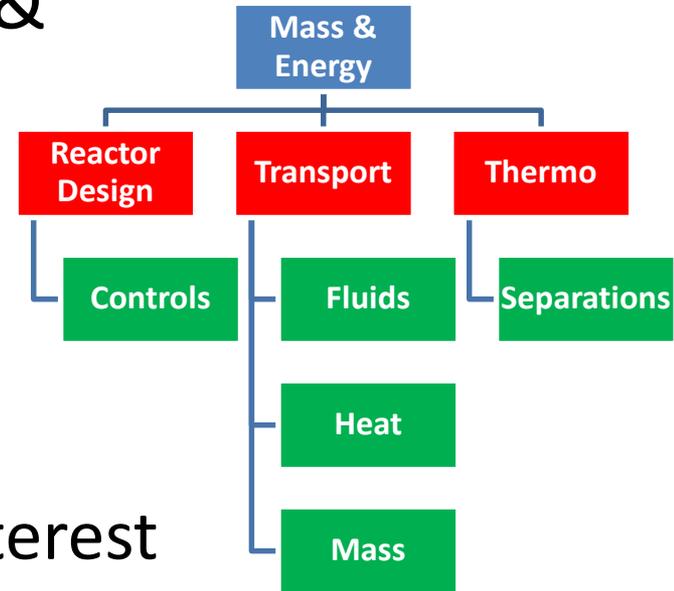
David
Himmelblau



A Vertical Integration of ChemE Education is Possible

- **Blur the lines between subjects & decompartmentalize knowledge**

- Emphasize “real” vs. “ideal”
- Facilitate retention of knowledge
- Give educators modern tools
- Open ChemE to anyone with an interest
- Make it exciting!



- **NEED: Deeply integrated sets of thermophysical properties, problem solving tools, graphing and data sharing capabilities**

Motivation behind the ChemE App

- 6 semesters teaching Mass & Energy Balances
- Lack of truly functional ChemE apps
 - Few selections/poor functionality
- Solving equations by hand takes time away from instruction
 - Look up values/constants in table, input into calculator or Excel, linear/double interpolations
- Want to rapidly (i.e. instantaneously) graph data
- ***ChemE needs tools that can do all of this***
 - ***And be visually attractive and enjoyable to use!***





Why iOS (Apple) Hardware?



- Survey of Mass & Energy Balance class showed strong student preference for Apple products
- Of those owning smartphones (71/75 students) >75% owned iPhones
- Of those owning tablets (*not* e-readers) (29/75 students), all but 2 were iPad
- ~90% of class has access to iOS platform in some form



Chemical Engineering AppSuite

- First launched on iPhone & iPod Touch – January 2012
 - v. 2.1 Aug. 21, 2013
- Features
 - Properties for 1000+ compounds
 - Converters for a variety of units
 - Integrated to automatically solve equations in any units
 - Steam tables
 - Also R134-a, Ammonia & Air
 - Equations of State
 - PR, RK, vdW, SRK, compressibility
 - Antoine Equation, Heat Capacity, Pressure Head
 - Delivery of reference material as PDFs



Example iPhone Screenshots

Verizon 3:33 PM

Back **octane**

octane
Compound

n-octane
Common Names

C₈H₁₈
Formula

111-65-9
CAS Number

[View in Wikipedia](#)

Verizon 3:28 PM

Back **Pressure**

atm

mm Hg

bar

Torr

psi

Verizon 3:32 PM

Back **Antoine Equation**

Antoine

neon

P: mm Hg

T: °F

Vapor Pressure

Verizon 3:34 PM

Back

114.23
Molecular Weight

0.703
Density (g/mL) at

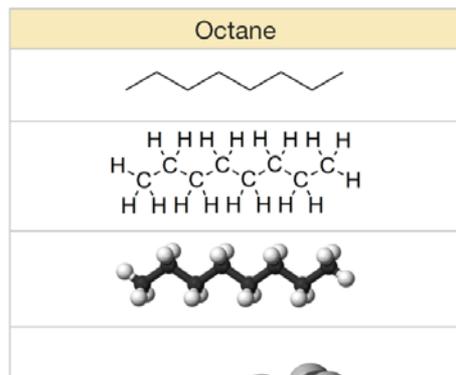
-56.8
Melting Temperature

125.6
Boiling Temperature

Octane

For the gasoline rating system, see [octane rating](#). For other uses, see [Octane \(disambiguation\)](#).



Verizon 3:30 PM

Back **Steam**

Saturated Superheated

T: K

P: atm

Phase: vapor

Cp: 2.162 kJ/kg-K

Cv: 1.615 kJ/kg-K

Density: 4.072 kg/m³

Enthalpy: 3012 kJ/kg

4415

7704

54

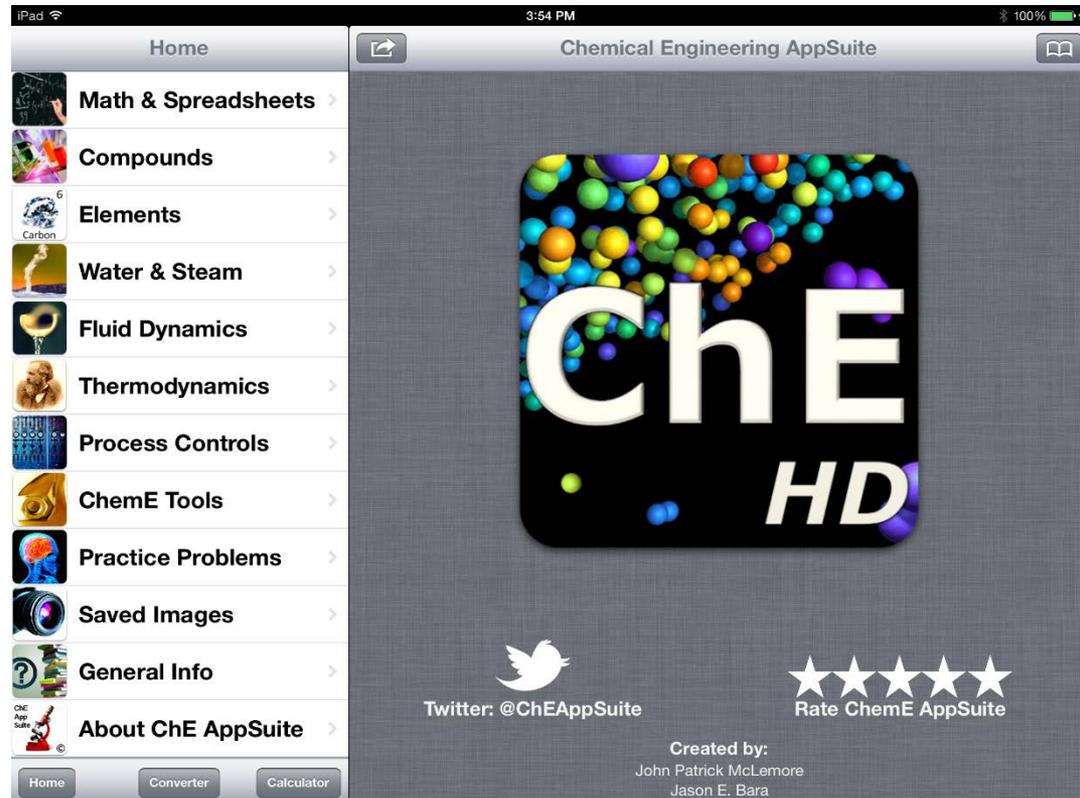
Chemical Engineering AppSuite HD

- Chemical Engineering App – Launched May 2012

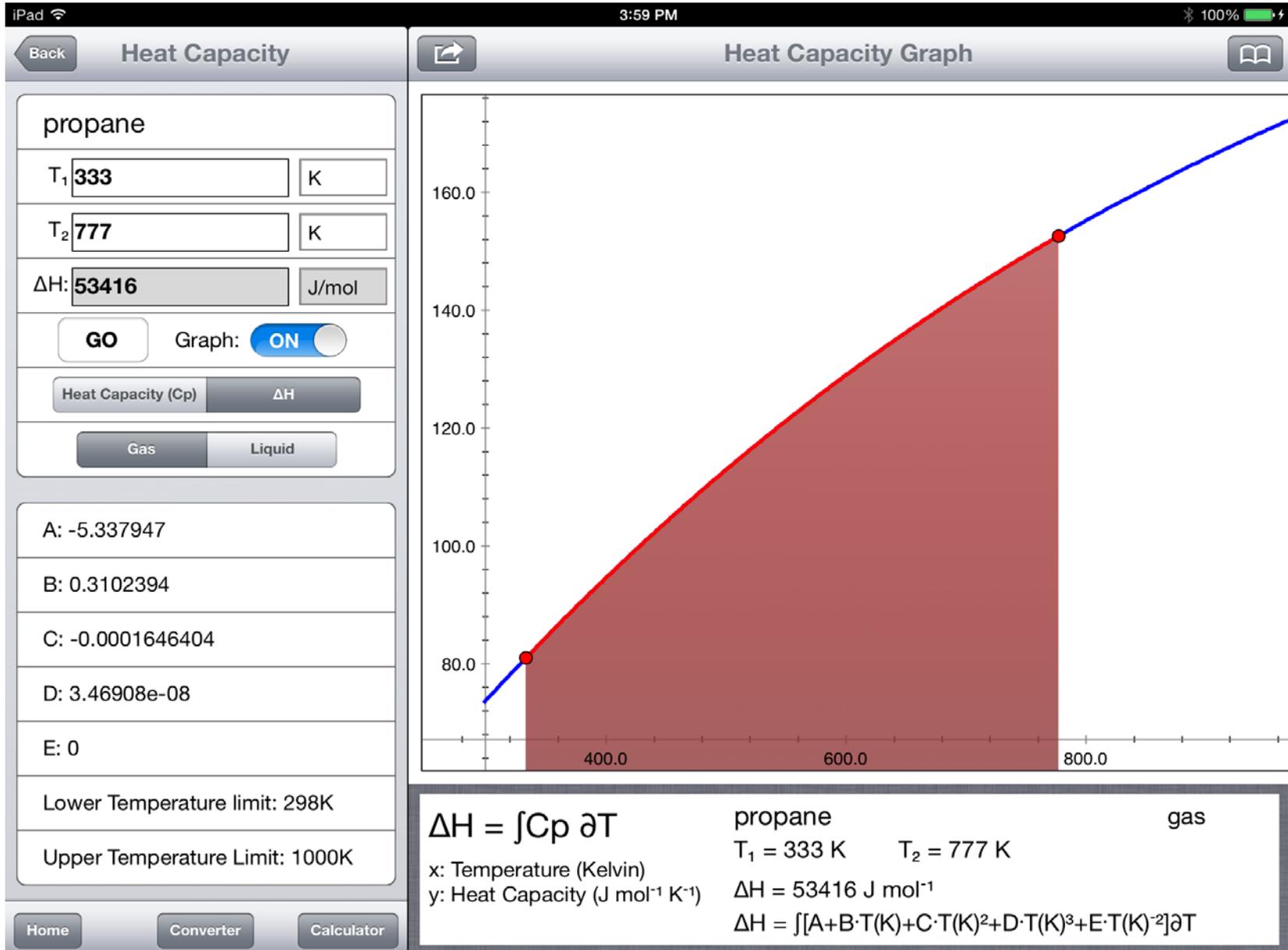
- Designed for iPad
- v. 2.1 Aug. 21, 2013

- Features

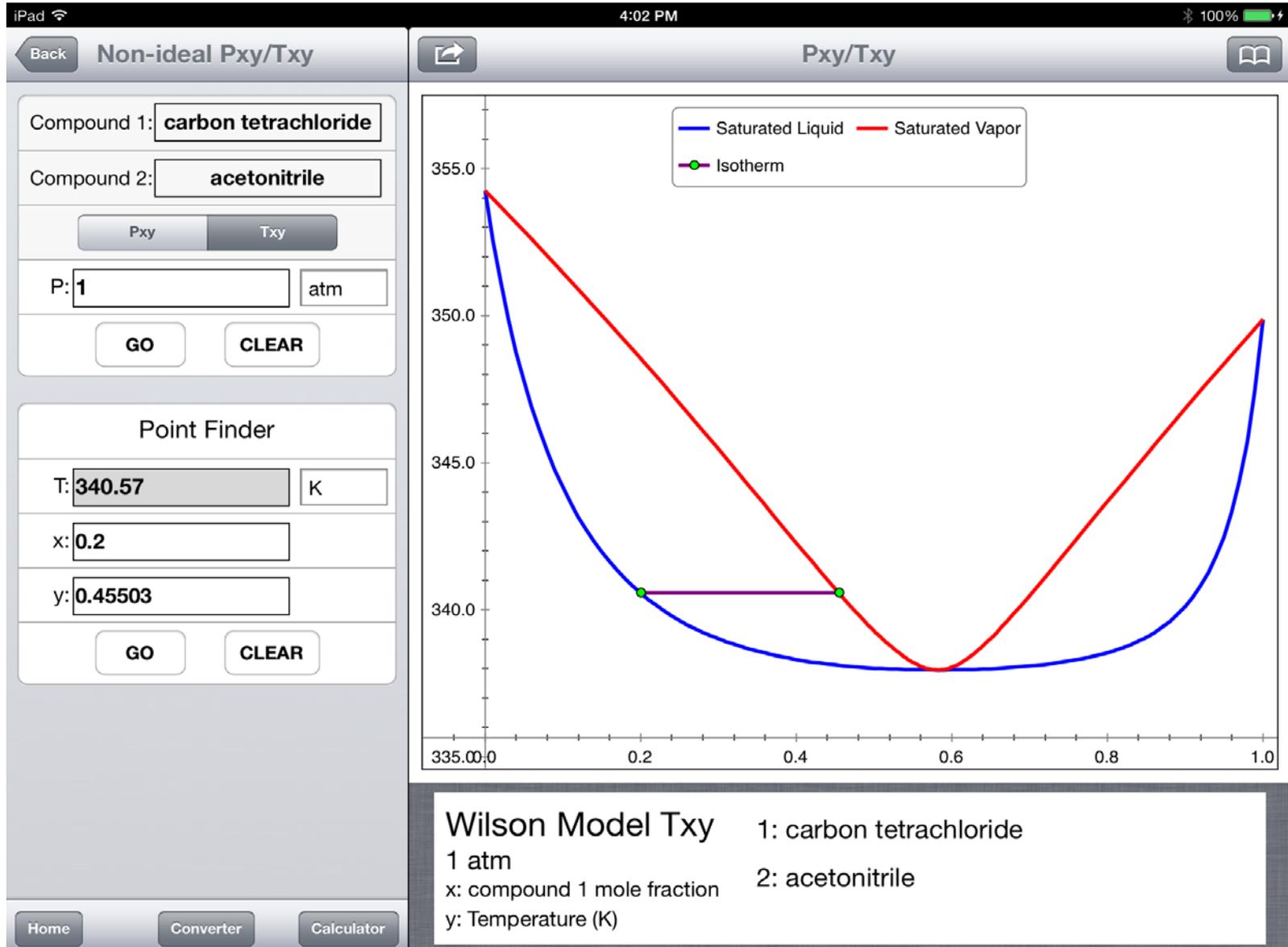
- All of iPhone functions
- **Graphing**
- VLE calculation
 - Raoult & Wilson
- Newtonian Fluids
- Matrix Operations
- Spreadsheets, Calculator
- “ChemE Tools”
- Practice Problems
- Ability to save work
- Integration with Twitter and email



iPad – Heat Capacity & ΔH



iPad – Wilson Model Txy Diagram



iPad – Combustion Analyzer

iPad 4:21 PM 100%

Back iPad Tools

Mass to Mole Converter >

Combustion Analyzer >

Tank Filling >

Polymer MW >

Home Converter Calculator

Combustion Analyzer

Choose Fuel 1 Fuel 1: octane

$C_8H_{18} + 12.5O_2 \rightarrow 8 CO_2 + 9 H_2O$ Fuel 1 moles: 12

CO formed? No Yes Fuel 1 frac. conv (f_1): .98

$C_8H_{18} + 8.5O_2 \rightarrow 8 CO + 9 H_2O$ Fuel 1 CO/(CO+CO₂): .125

Get Theoretical Oxygen theoretical O₂ (moles): 150

Combustion Conditions

Air Pure Oxygen Custom

% excess air/O₂: 25 mole fraction O₂: 0.21 mole fraction N₂: 0.79

other inerts present? No Yes none moles inerts

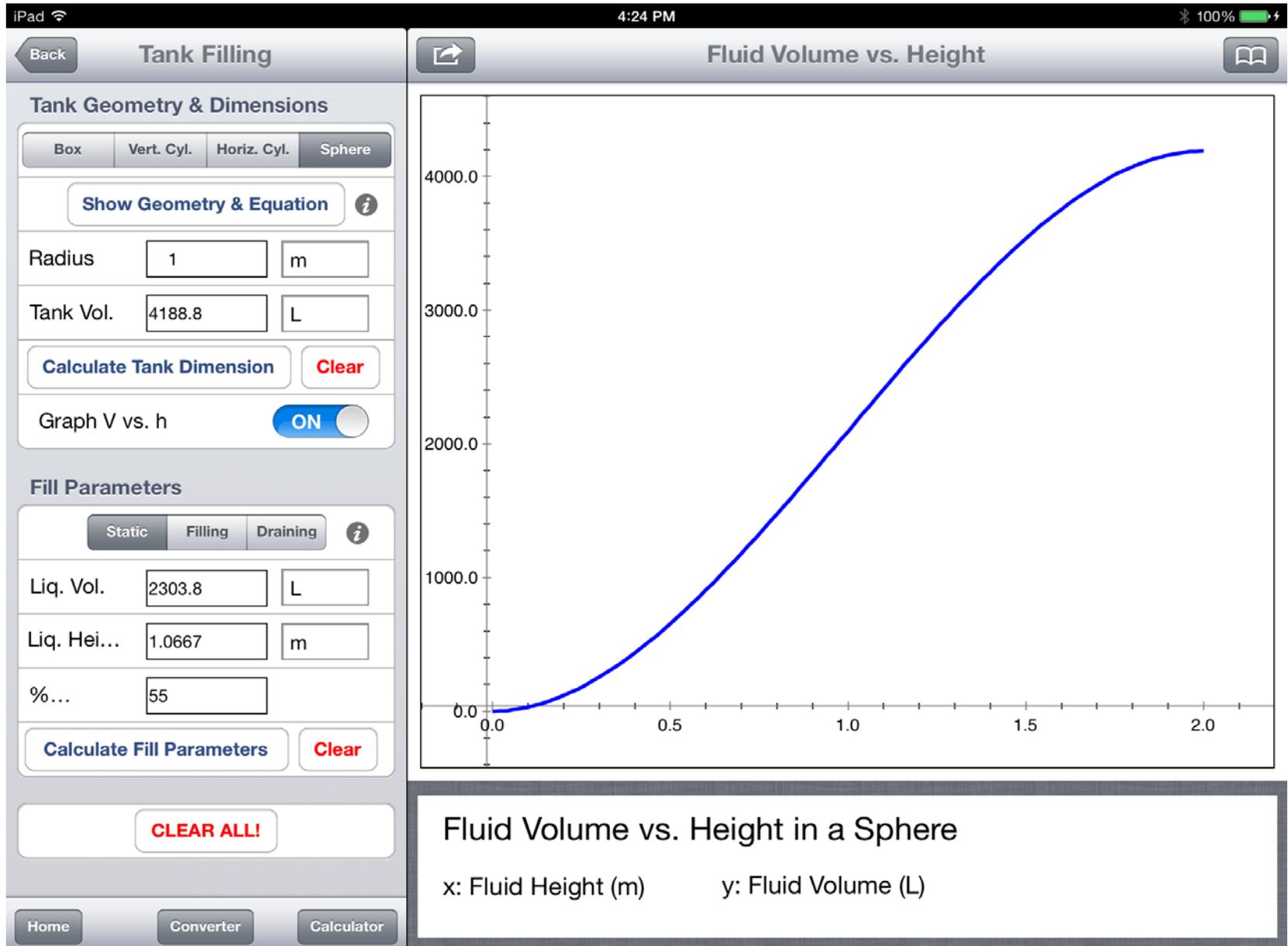
Get Inlet Composition

Inlet Composition

	n_i (moles)	y_i (mol frac.)
Fuel 1: C ₈ H ₁₈	12	0.01326
O ₂	187.5	0.2072
N ₂	705.36	0.7795
Total	904.86	1



iPad – Tank Filling



iPad – Tank Filling

iPad 4:23 PM 100%

Tank Filling

Back

Tank Geometry & Dimensions

Box Vert. Cyl. Horiz. Cyl. **Sphere**

Show Geometry & Equation *i*

Radius m

Tank Vol. L

Calculate Tank Dimension **Clear**

Graph V vs. h

Fill Parameters

Static **Filling** Draining *i*

Liq. Vol. L

Liq. Hei... m

%...

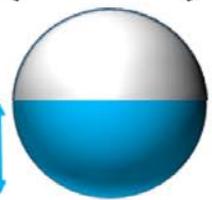
Calculate Fill Parameters **Clear**

CLEAR ALL!

Home Converter Calculator

Sphere

Diameter = 2x Radius (r)

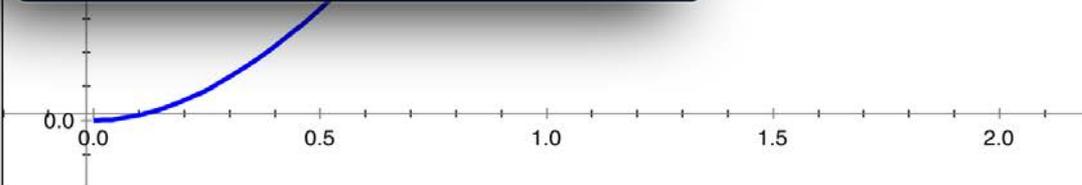


Fluid Height (h_f)

Overall Tank Volume:

$$V_f = \frac{4\pi}{3} r^3$$

Fluid Volume at a Given Fluid Height:

$$V_f = \frac{\pi}{3} h_f^2 (3r - h_f)$$


ChE HD

Fluid Volume vs. Height in a Sphere

x: Fluid Height (m) y: Fluid Volume (L)

ChE HD



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



iPad – Mixer Practice Problem

iPad
4:06 PM
100%

Practice Problems **Calculator**

.6938×833+.9259×663
▶ 1191.8071
■ 1191.8/1496
▶ 0.79665774

2nd CLEAR DEL ABOUT
sin cos tan avg
sinh cosh tanh stddev
ln e^ log 10^
! % π EE
^ ^2 ()
√ , / ×
7 8 9 -
4 5 6 +
1 2 3 =
0 . ans

Calculator Graphing Graph Data

2 Component Mixer

Two streams containing mixtures of A and B are combined to produce a single stream. Using the data given below, calculate the masses of each stream and the mass fractions of each component in each stream.

Mixing Tank

	mass (m_i)	mass frac. A (x_i^A)	mass frac. B (x_i^B)
Stream 1	<input type="text" value="833"/>	<input type="text" value=".6938"/>	<input type="text" value="0.3062"/>
Stream 2	<input type="text" value="663"/>	<input type="text" value=".9259"/>	<input type="text" value="0.0741"/>
Stream 3	<input type="text" value="1496"/>	<input type="text" value=".7967"/>	<input type="text" value=".2033"/>

correct

of attempts, this problem:

times solved overall:



iPad - Reference PDFs



Simplified Psychrometric Chart - SI Units

Enthalpy at Saturation (kJ / kg dry air)

Wet Bulb or Saturation Temperature (°C)

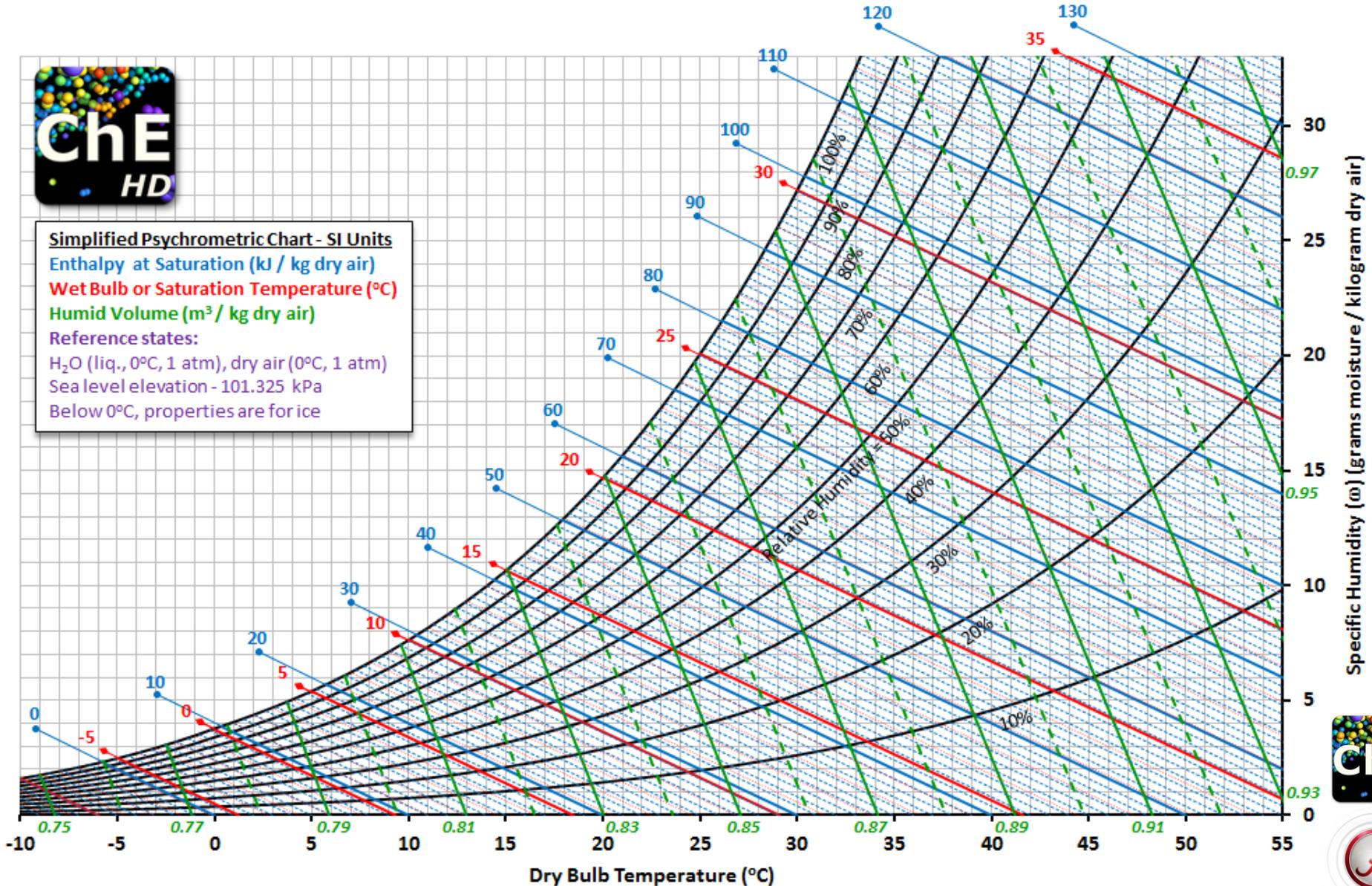
Humid Volume (m³ / kg dry air)

Reference states:

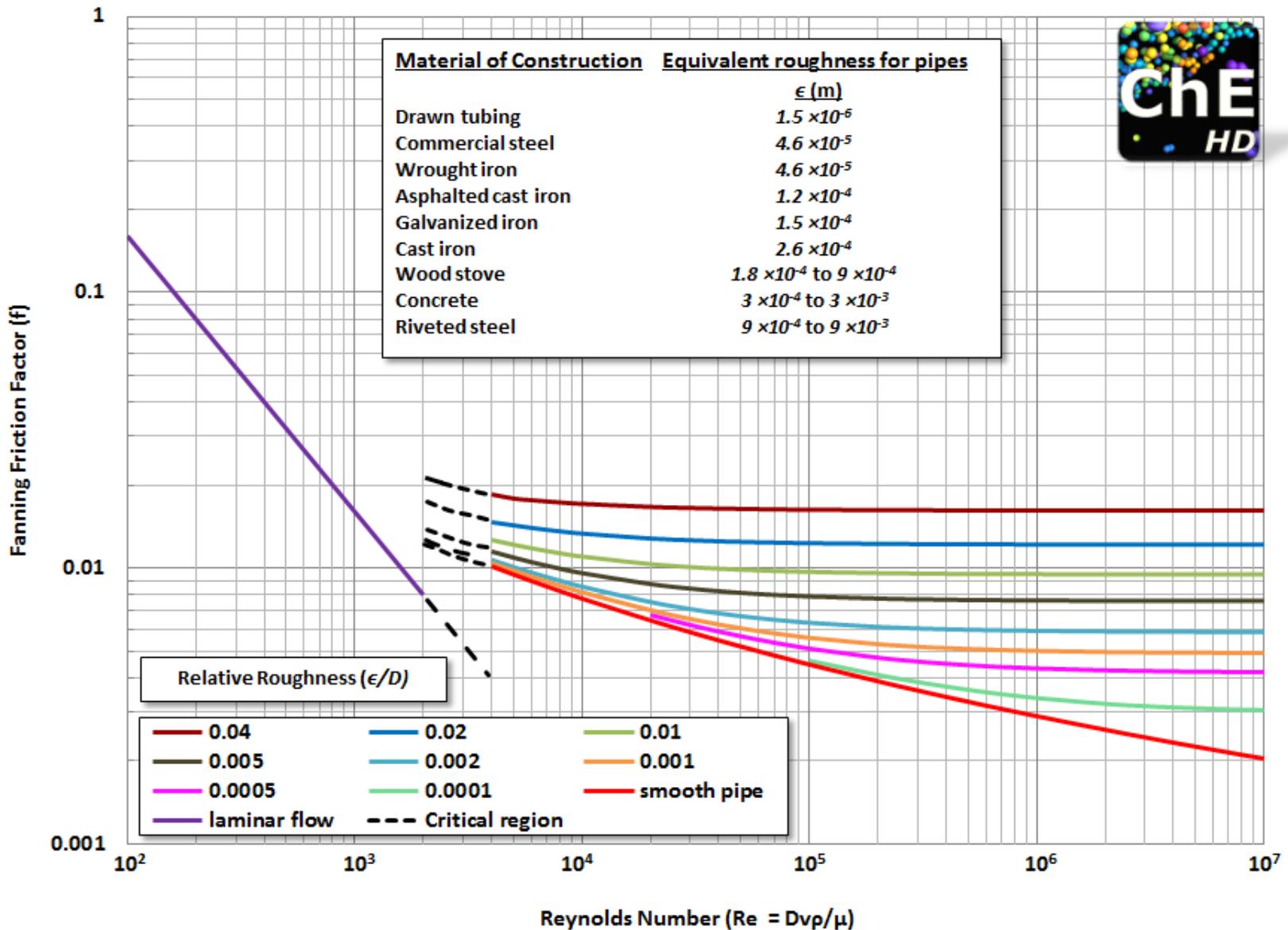
H₂O (liq., 0°C, 1 atm), dry air (0°C, 1 atm)

Sea level elevation - 101.325 kPa

Below 0°C, properties are for ice



iPad - Reference PDFs



Student Response

- Students have been overwhelmingly enthusiastic about using their iPhones and iPads to solve problems in class
 - Most had not considered these devices in this light
 - View technology primarily for entertainment/communications



- Appreciate accessibility of spreadsheet, matrix tools
 - Students can be intimidated by Excel, Matlab
- Enjoy learning about advanced concepts before taking Thermo, Fluids, etc.

Challenges & Opportunities

- Not all students have iPhones and/or iPads
 - Can we require an iPad in the ChemE curriculum?
 - Some cite cost as a barrier (\$500+), but iPad mini and used devices can lower activation energy (< \$350)
- How user-friendly should the software be?
 - Do we allow users to input “bad” values
 - i.e. mass fraction > 1
- Great for well-defined equations but can we make it more open-ended?
 - Parametric analysis in mass & energy balances?
 - Process simulation modules?



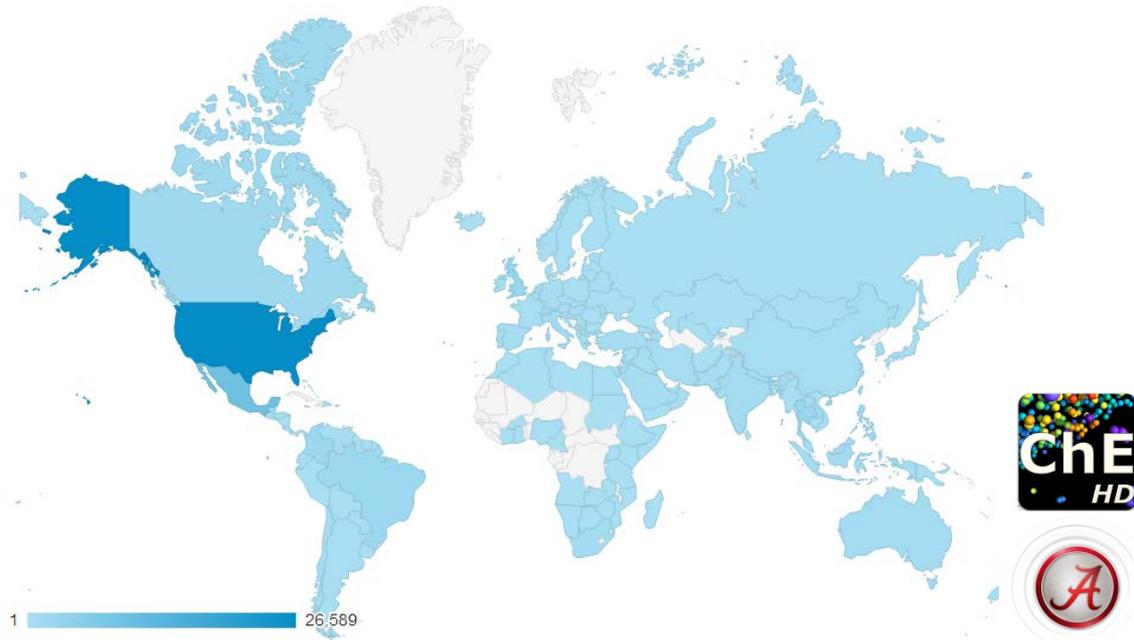
Teaching Benefits

- A mobile approach saves time!
 - More rapid equation solving and data retrieval
 - iPad can be displayed on projector
- Students are excited by the visuals
 - See the behavior of functions vs. temp, shapes of molecules
 - Appeal to different learning styles
- Enhance content in mass & energy balances
 - Pull in concepts from thermodynamics, separations
 - e.g. rapidly compare ideal gas law to other EOS
 - e.g. basic principles of stages in distillation columns



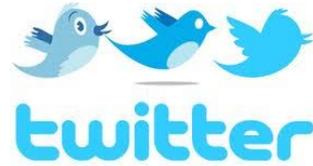
A Global Impact

- Since release of v. 2.0 on May 15, 2013:
 - App utilized by > 15,500 users > 67,000 times
 - More than 4200 cities in 153 countries
 - Facilitated > 225,000 calculations
- U.S. is #1 country of use (~40%), but top 6 cities are:
 - Mexico City
 - Tuscaloosa 
 - Monterrey, MX
 - Bangkok
 - Bogota
 - Houston



Current & Near Future Plans

- Continue to build a user base
 - App exposure still limited, but growth is accelerating
 - Actively communicate with and get feedback from users



@ChEAppSuite

- Consolidate thermophysical property interfaces
 - Expedite calculations of dimensionless groups, etc.
- EOS for mixtures
- Expand practice problems to provide a full course of study in Mass & Energy Balances





Thank You!

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