



# Chemical Engineering App:

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

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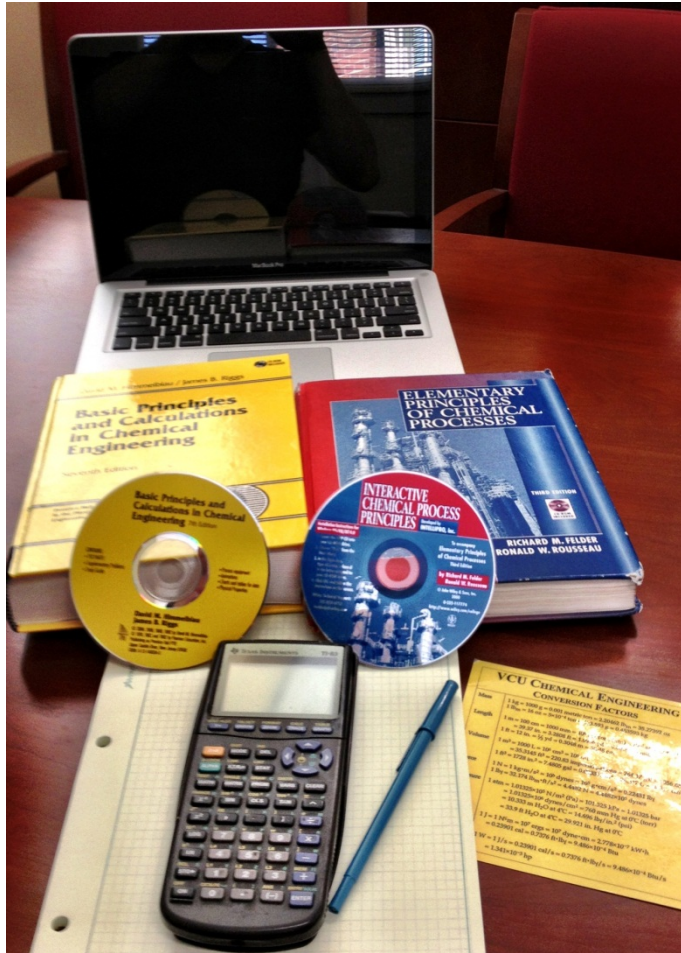
AIChE Annual Meeting  
San Francisco, CA  
November 6, 2013

# 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...*

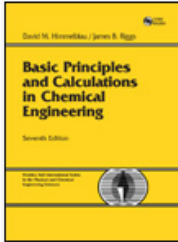


*Can we do more with less?*

# 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 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 skills

#### Charts

- [Compressibility Charts](#)—compressibility charts that can be used to determine the compressibility factor
- [Psychrometric Charts](#)—two psychrometric charts that can be used to determine the humidity ratio and the wet-bulb temperature

#### Process Equipment

The screenshot shows a software window titled "Chemical Engineering" with a menu bar containing "Physical Properties", "Heat Capacities", "Enthalpies", "Density of Liquid", "Vapor Pressure", and "Steam Tables". The "Physical Properties" menu is selected. On the left, there is a list of compounds under "Miscellaneous" and "Formula" categories. "AMMONIA" is selected in the "Miscellaneous" list. On the right, the properties for "AMMONIA" are displayed in a table format.

Property	Value
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 (cm <sup>3</sup> /mol)	72.5
Critical Density (g/cm <sup>3</sup> )	0.235
Critical Compressibility (Z <sub>c</sub> )	0.242
Ascentric Factor (ω)	0.25
Enthalpy of Formation (kJ/g mol) (at 298.15K)	-45.68928(g)
Enthalpy of Vaporization (kJ/g mol) (at normal boiling point)	23.251

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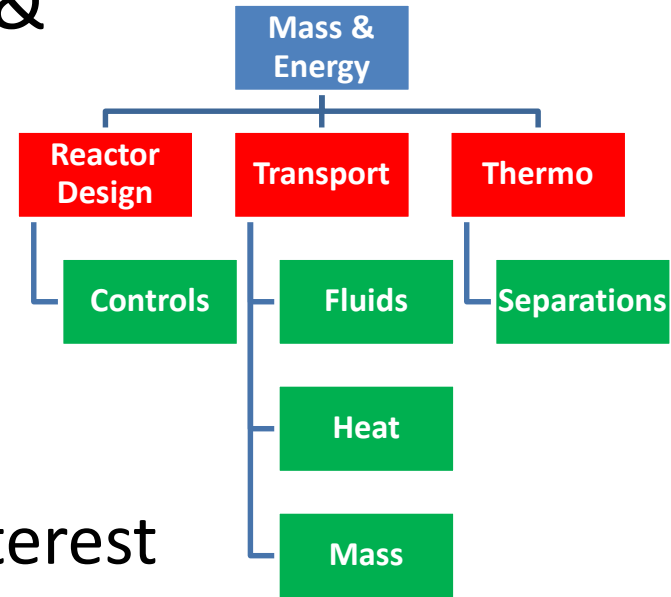
David  
matio



# 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

**C<sub>8</sub>H<sub>18</sub>**  
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   ΔHvap

Verizon 3:34 PM

Back




**114.23**  
Molecular Weight

**0.703**  
Density (g/mL) at

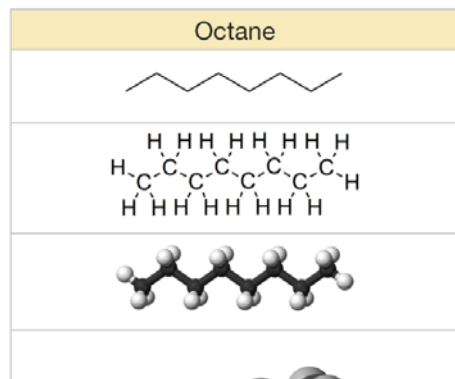
**-56.8**  
Melting Temperature

**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

GO   Clear

Phase: vapor

Cp: 2.162 kJ/kg-K

Cv: 1.615 kJ/kg-K

Density: 4.072 kg/m<sup>3</sup>

Enthalpy: 3012 kJ/kg

GO

4415

7704

54



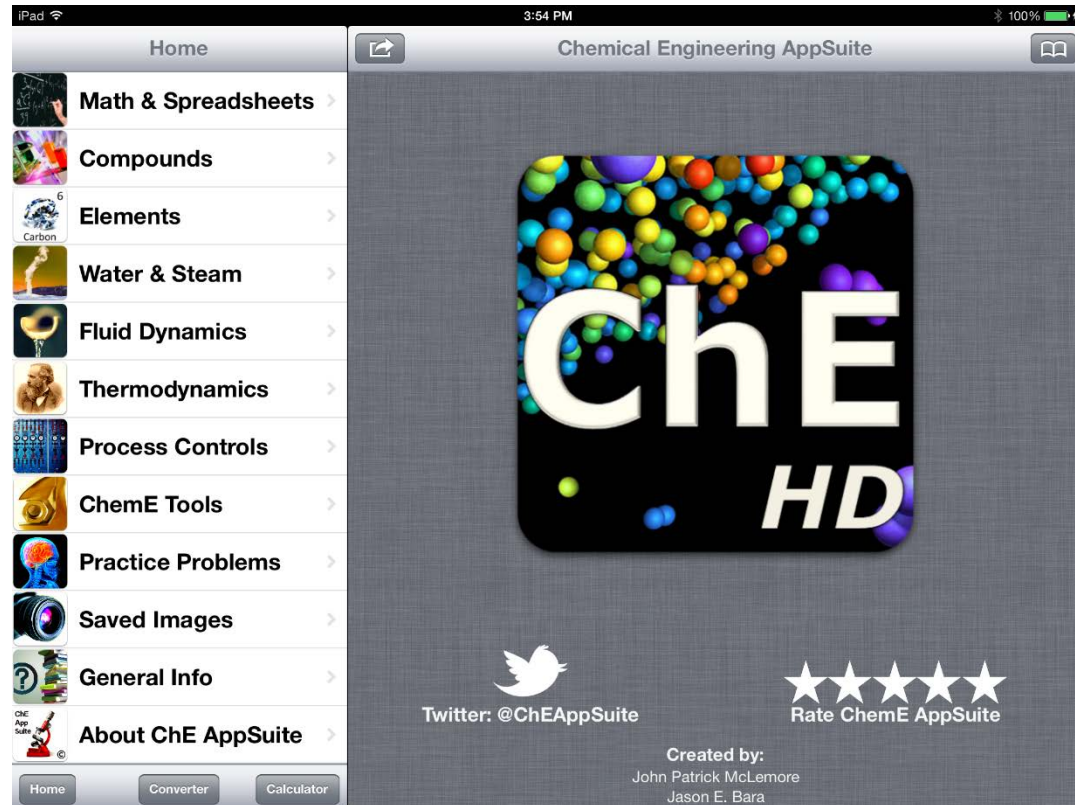
# Chemical Engineering AppSuite HD

- Chemical Engineering App – Launched May 2012

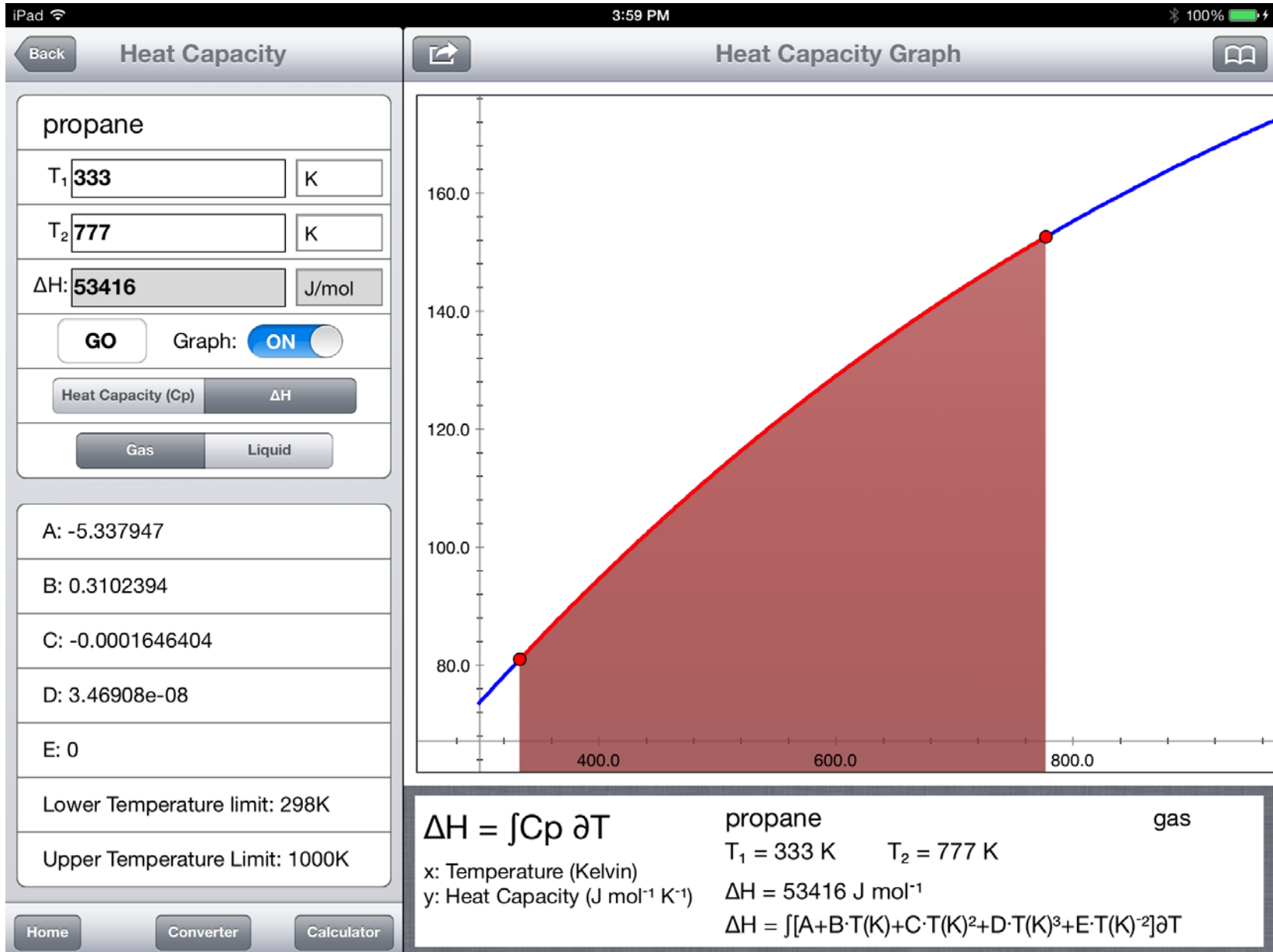
- Designed for iPad
- v. 2.1 Aug. 21, 2013

- Features

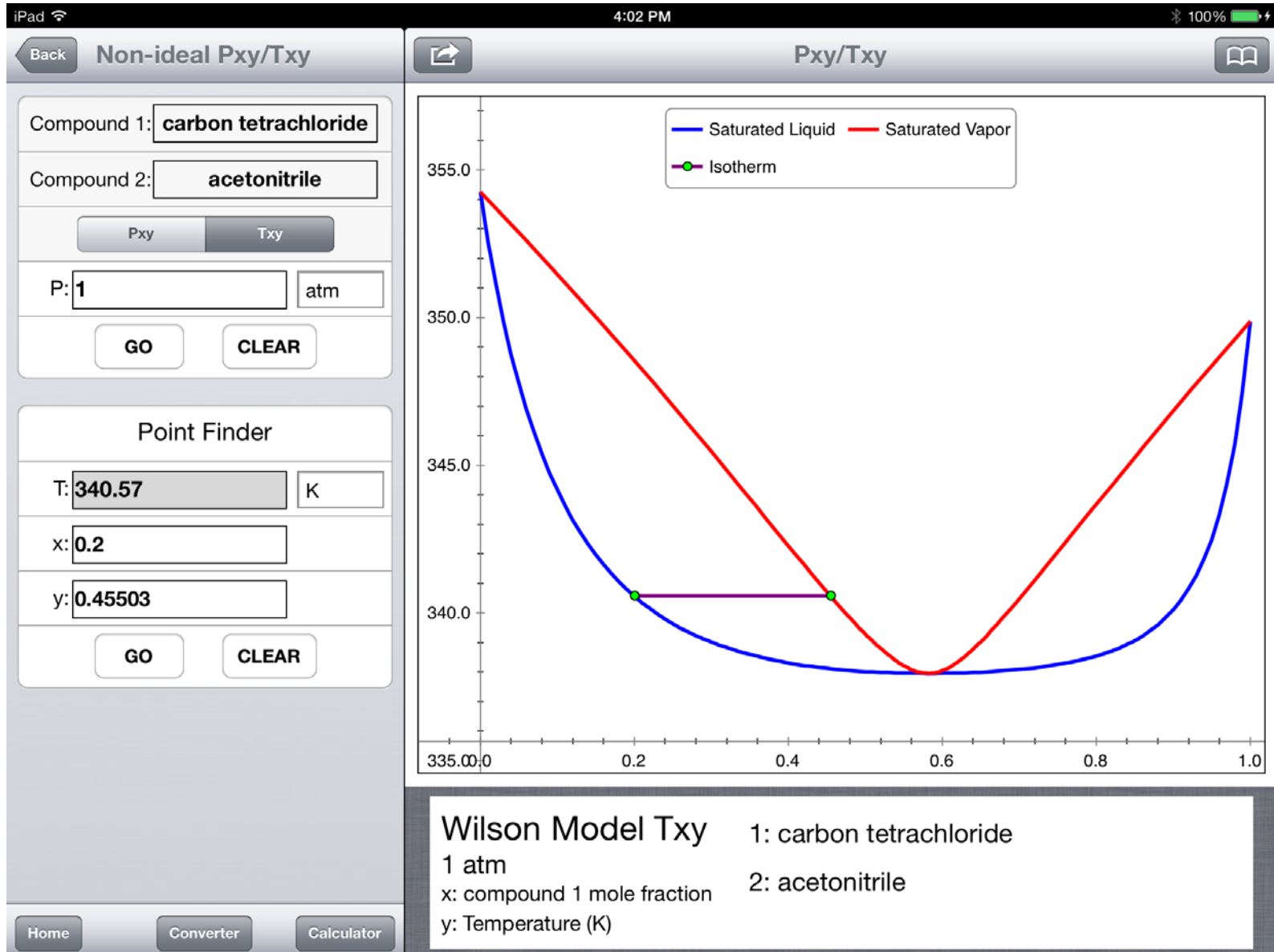
- All of iPhone functions
- **Graphing**
- VLE calculation
  - Raoult & Wilson
- Newtonian Fluids
- Matrix Operations
- Spreadsheets, Calculator
- “ChemE Tools”
- Practice Problems
- Ability to save work
- Integration with Twitter and email



# iPad – Heat Capacity & $\Delta H$



# 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+CO<sub>2</sub>): .125

Get Theoretical Oxygen theoretical O<sub>2</sub> (moles): 150

### Combustion Conditions

Air Pure Oxygen Custom

% excess air/O<sub>2</sub>: 25 mole fraction O<sub>2</sub>: 0.21 mole fraction N<sub>2</sub>: 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 <sub>8</sub> H <sub>18</sub>	12	0.01326
O <sub>2</sub>	187.5	0.2072
N <sub>2</sub>	705.36	0.7795
Total	904.86	1



# iPad – Tank Filling

iPad 4:24 PM 100%

## Tank Filling

### Fluid Volume vs. Height

**Tank Geometry & Dimensions**

Box Vert. Cyl. Horiz. Cyl. Sphere

Show Geometry & Equation

Radius: 1 m

Tank Vol.: 4188.8 L

Calculate Tank Dimension Clear

Graph V vs. h ON

**Fill Parameters**

Static Filling Draining

Liq. Vol.: 2303.8 L

Liq. Hei...: 1.0667 m

%...: 55

Calculate Fill Parameters Clear



CLEAR ALL!

Home Converter Calculator

Fluid Height (m)	Fluid Volume (L)
0.0	0.0
0.5	~600.0
1.0	~2000.0
1.5	~3500.0
2.0	4188.8

Fluid Volume vs. Height in a Sphere

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



# iPad – Tank Filling

iPad 4:23 PM 100%

## Tank Filling

Back

### Tank Geometry & Dimensions

Box Vert. Cyl. Horiz. Cyl. Sphere

Show Geometry & Equation

Radius 1 m

Tank Vol. 4188.8 L

Calculate Tank Dimension Clear

Graph V vs. h ON

### Fill Parameters

Static Filling Draining

Liq. Vol. 2303.8 L

Liq. Hei... 1.0667 m

%... 55

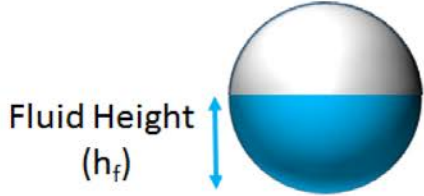
Calculate Fill Parameters Clear

CLEAR ALL!

Home Converter Calculator

### Sphere

Diameter = 2x Radius (r)

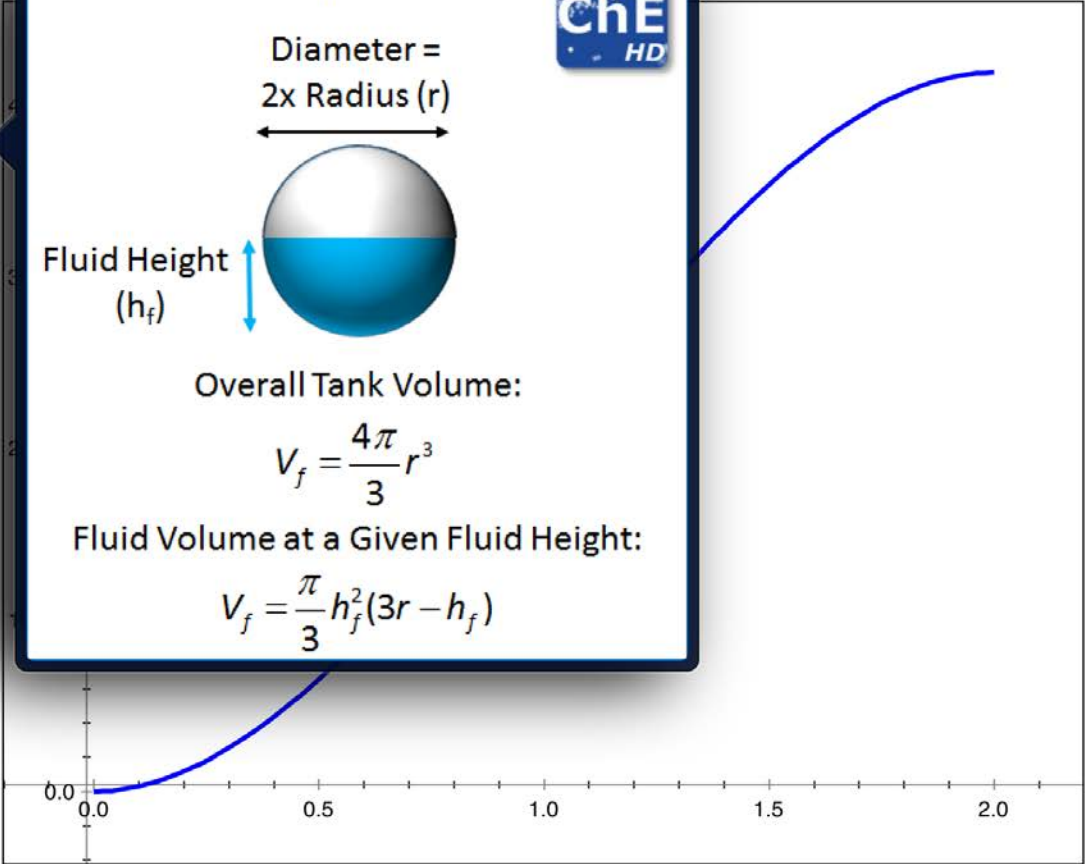


Fluid Height ( $h_f$ )

Overall Tank Volume:

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



Fluid Volume at a Given Fluid Height:

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


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.

	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)

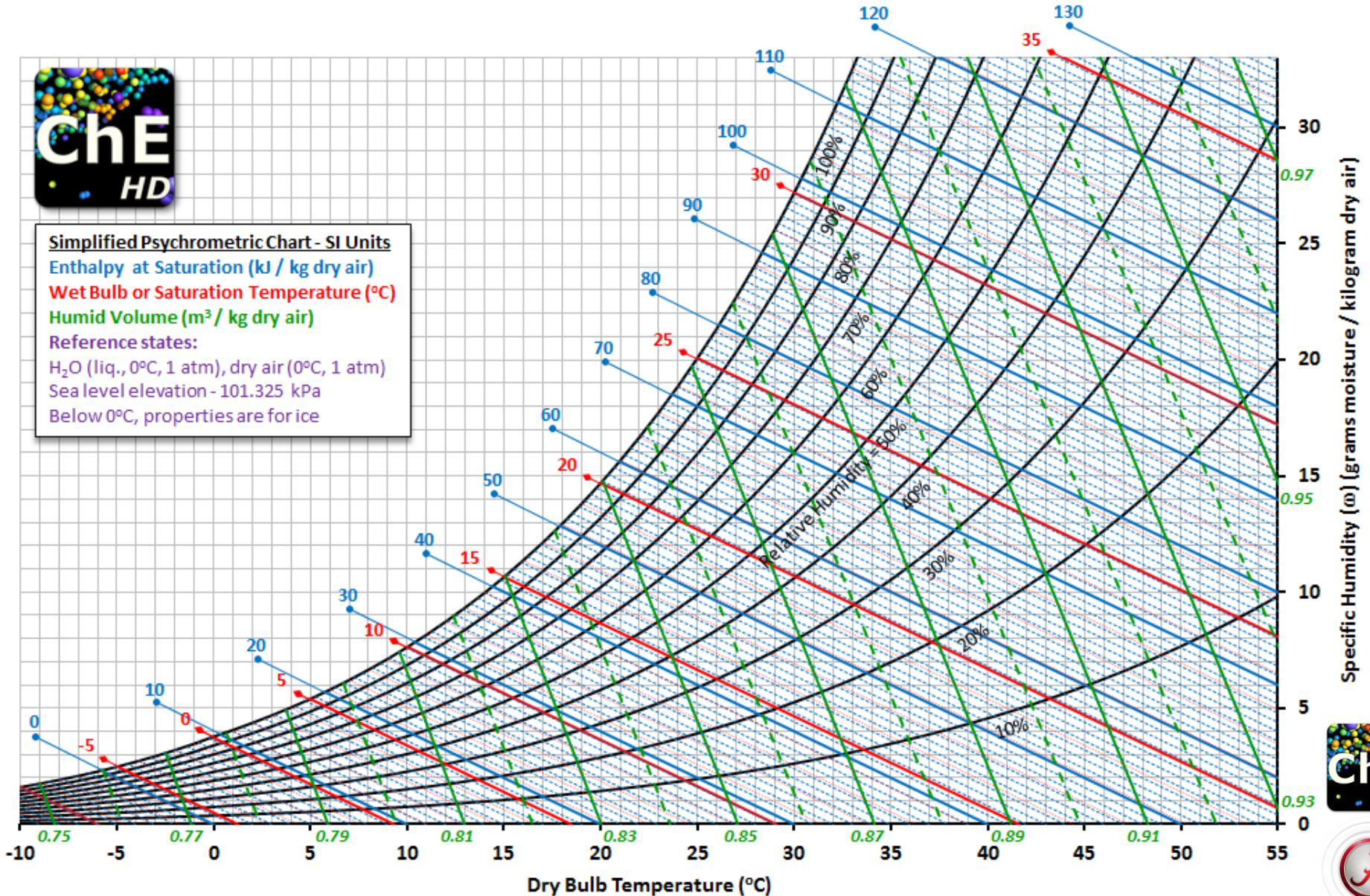
Humid Volume (m<sup>3</sup> / kg dry air)

Reference states:

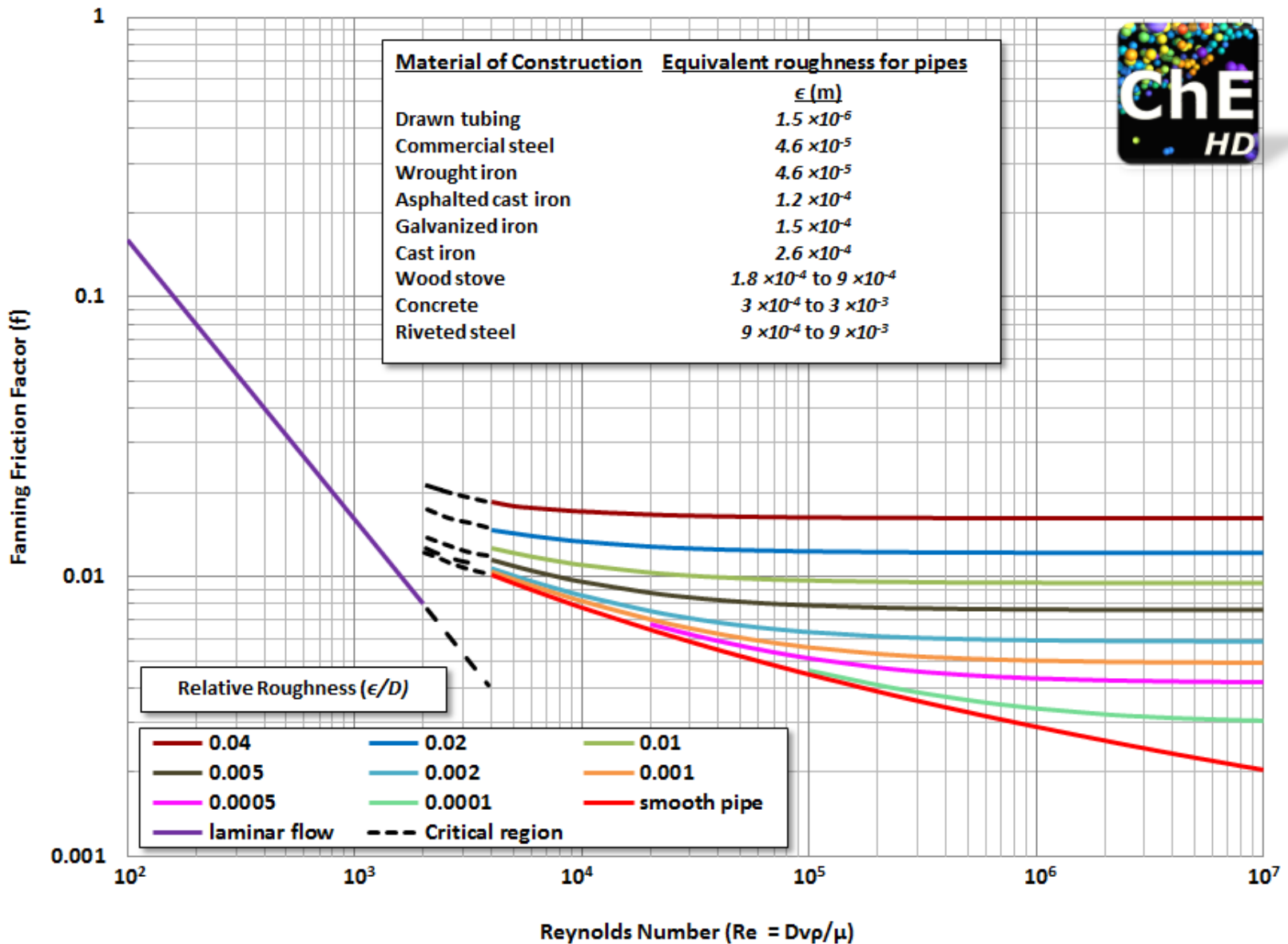
H<sub>2</sub>O (liq., 0°C, 1 atm), dry air (0°C, 1 atm)

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?




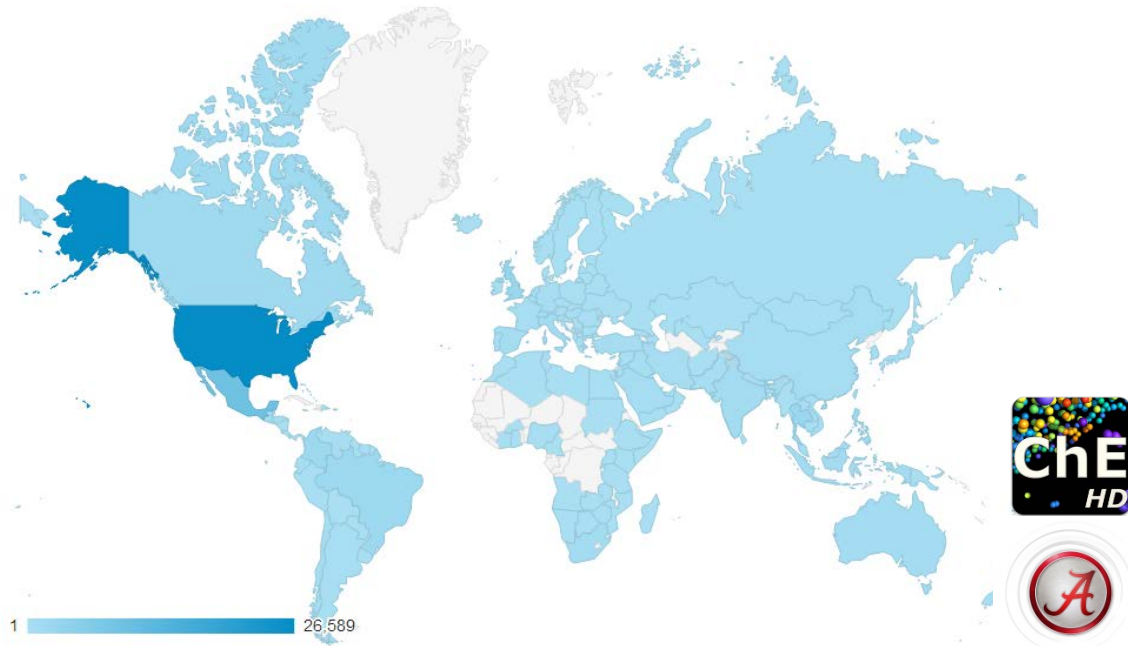
# Teaching Benefits

- 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



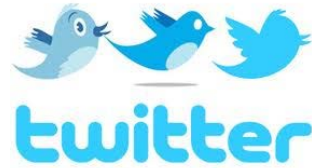
# A Global Impact

- 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](https://twitter.com/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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