Integrating Virtual Labs into the AP/IB Chemistry Curriculum

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Science By Simulation

www.sciencebysimulation.com

Questions

- What are virtual labs?
- How do they align with AP/IB chemistry?
- How can I set up & run virtual experiments?
- Why should I use virtual labs?
- How can I assign and assess virtual labs?

What are virtual labs?

- Based on simulation tools & technologies
- Common in industry, still new to academia
- Run experiments through a web browser
- Easy to generate data and report results

Simulation tools used

- Two web apps, both available free:
  - **ChemReaX**™: chemical reaction simulator
    - www.sciencebysimulation.com/chemreax
  - **GasSim**™: gas law simulator
    - www.sciencebysimulation.com/gassim

Demonstration topics

- **Equilibrium**
  - Effect of temperature/pressure changes (Le Chatelier's principle)
  - AP: unit 10; IB: unit 7
- **Kinetics**
  - Reaction order, rate constant, half life
  - AP: unit 9; IB: unit 6
- **Acid-Base Titration**
  - Polyprotic acids, hydrolysis
  - AP: unit 11; IB: unit 8
- **Gas Laws**
  - Real gases, deviations from ideal gas law
  - AP: unit 4; IB: unit 1

Equilibrium

Effect of temperature, exothermic reaction

- **Reaction:** **Methanol synthesis**
  - $CO\ (g) + 2H_2\ (g) \rightleftharpoons CH_3OH\ (g)$

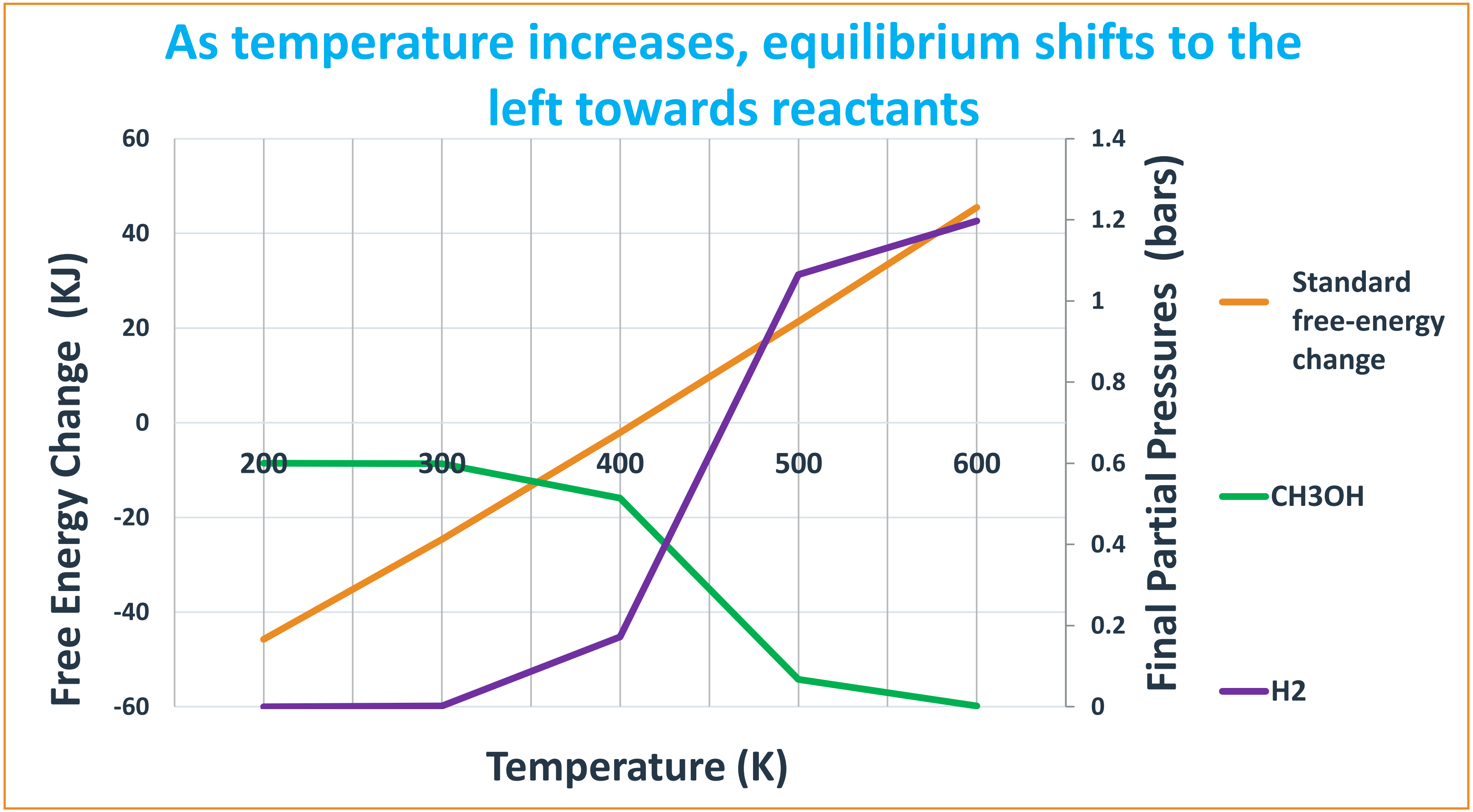
- **Virtual Experiment:**

ChemReaX

  - **Simulate the reaction in ChemReaX under different temperatures and collect data**
    - Initial partial pressures: P(CO) = 10 bar; P(H2) = 1 bar ; P(CH3OH) = 0.1 bar
  - **Plot the final composition and free energy vs. temperature**

Equilibrium

Effect of temperature, exothermic reaction



Equilibrium

Effect of temperature, endothermic reaction

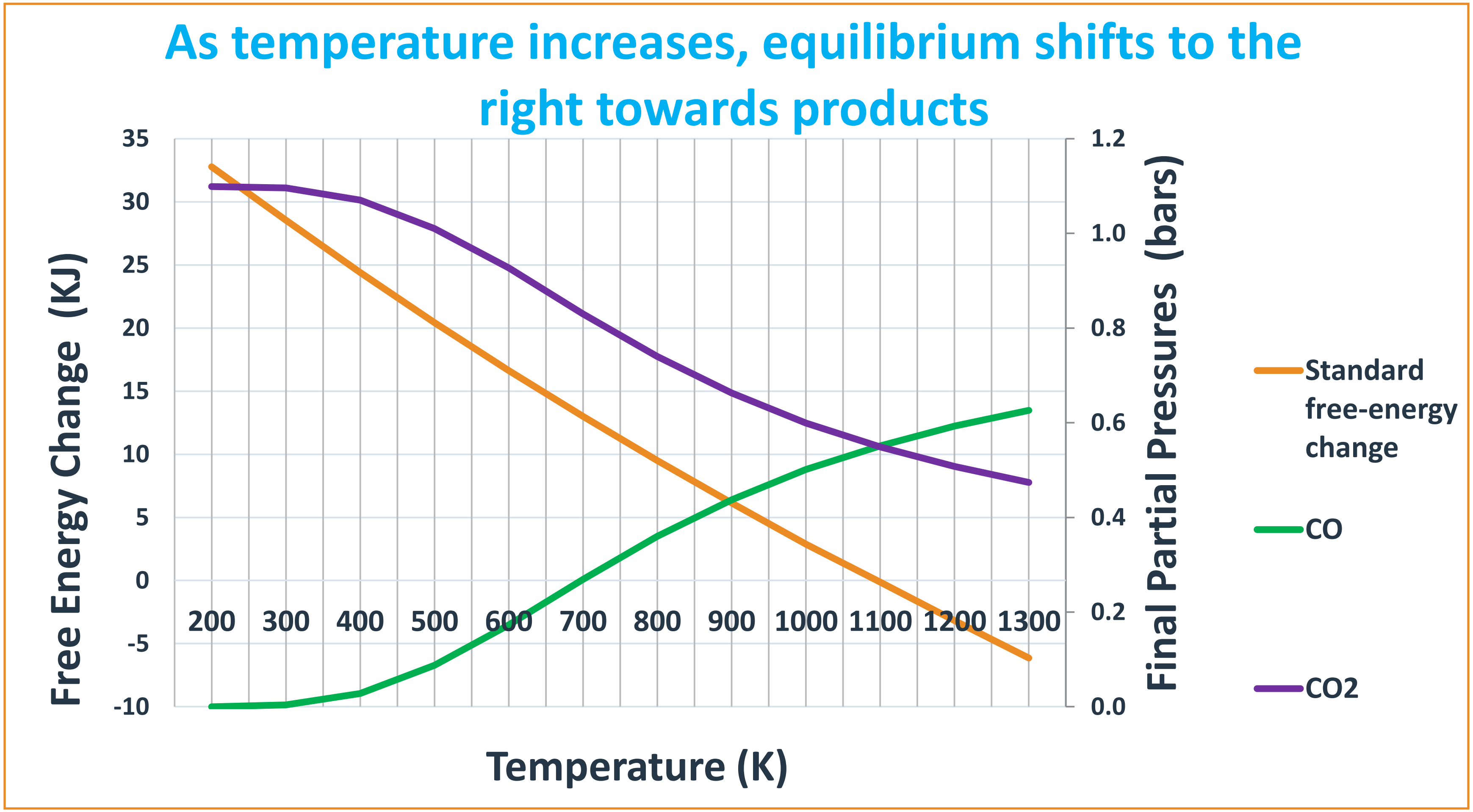
- **Reaction:**
  - $H_2\ (g) + CO_2\ (g) \rightleftharpoons H_2O\ (g) + CO\ (g)$
- **Virtual Experiment:**

ChemReaX

  - **Simulate the reaction in ChemReaX under different temperatures and collect data**
    - Initial partial pressures: P(H2) = P(CO2) = 1 bar; P(CO) = P(H2O) = 0.1 bar
  - **Plot the final composition and free energy vs. temperature**

Equilibrium

Effect of temperature, endothermic reaction



Equilibrium
Effect of pressure

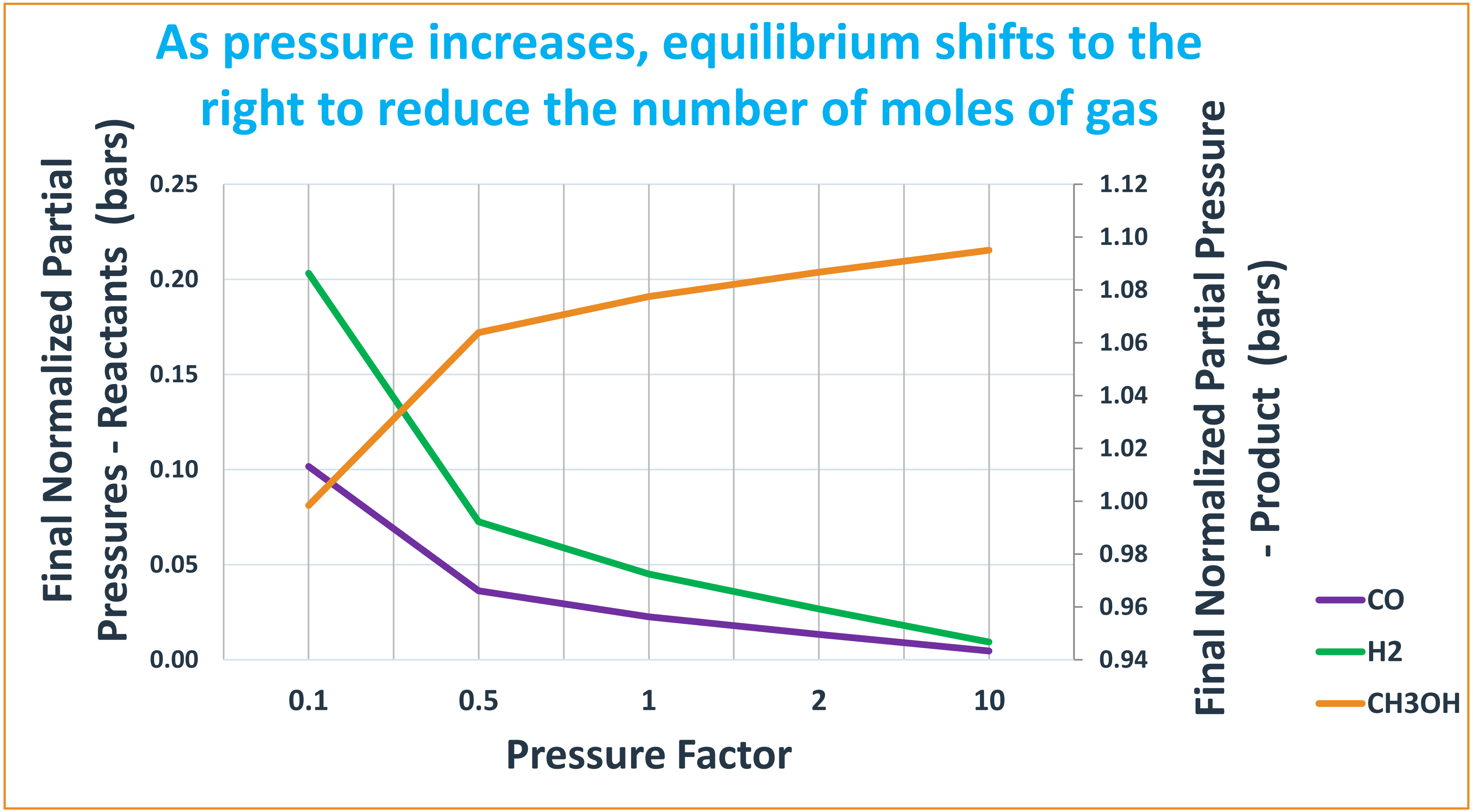
- **Reaction:**
  - $CO\ (g) + 2H_2\ (g) \rightleftharpoons CH_3OH\ (g)$

- **Virtual Experiment:**

ChemReaX

  - **Simulate the reaction in ChemReaX under different pressure factors and collect data**
    - Initial partial pressures: P(CO) = 1 bar; P(H2) = 2 bar; P(CH3OH) = 0.1 bar
  - **Plot the final composition vs. pressure factor**

Equilibrium
Effect of pressure



Kinetics

Effect of reaction order

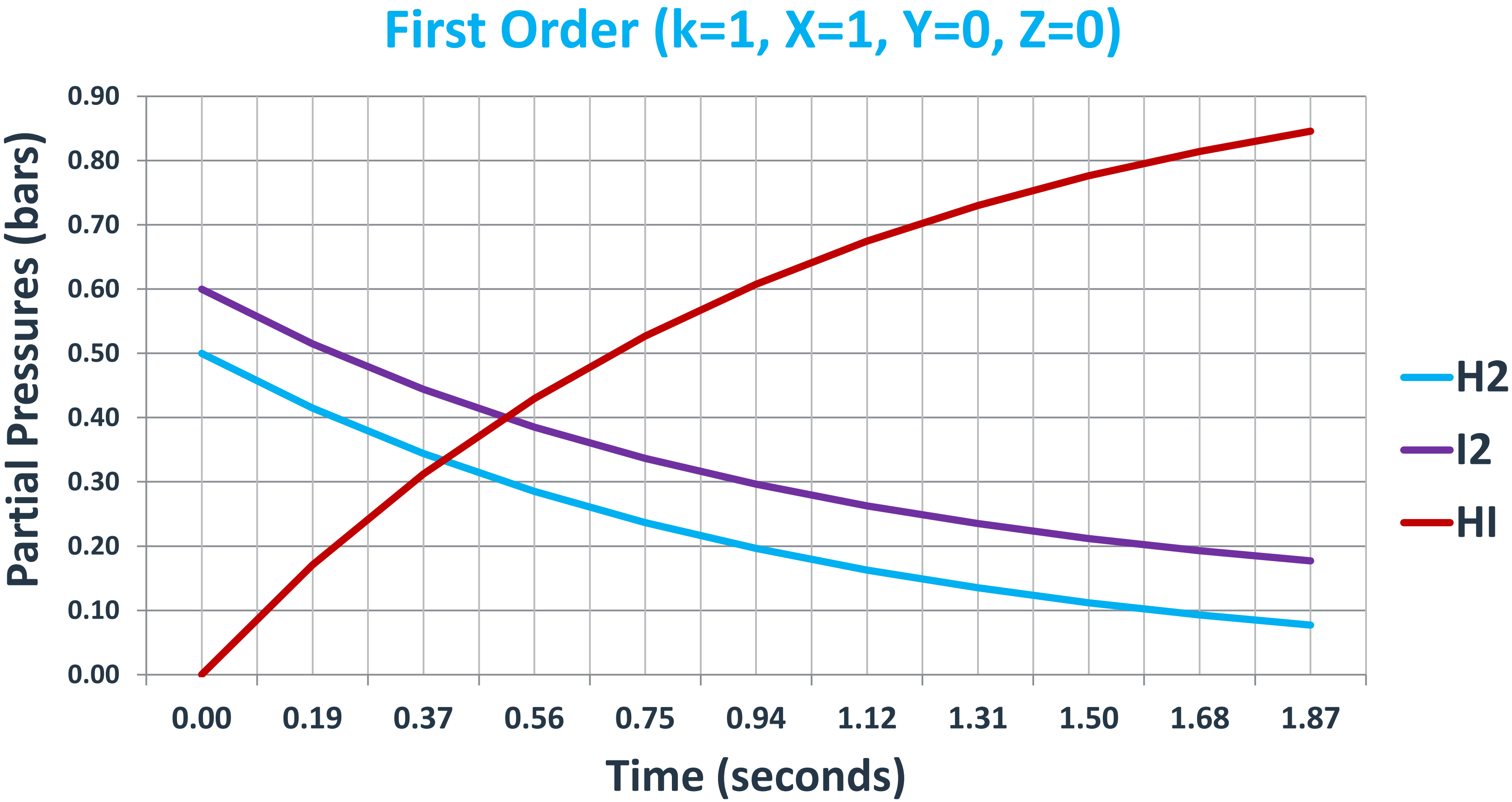
- **Reaction:**
  - **H_2 (g) + I_2 (g) ⇌ 2HI (g)**
- **Virtual Experiment:**

ChemReaX

  - **Simulate the reaction kinetics modeled as first/second/third order and collect data**
    - Initial partial pressures: P(H_2) = 0.5 bar; P(I_2) = 0.6 bar; P(HI) = 0
    - Temperature: 721K
  - **Plot the reaction progress vs. time**

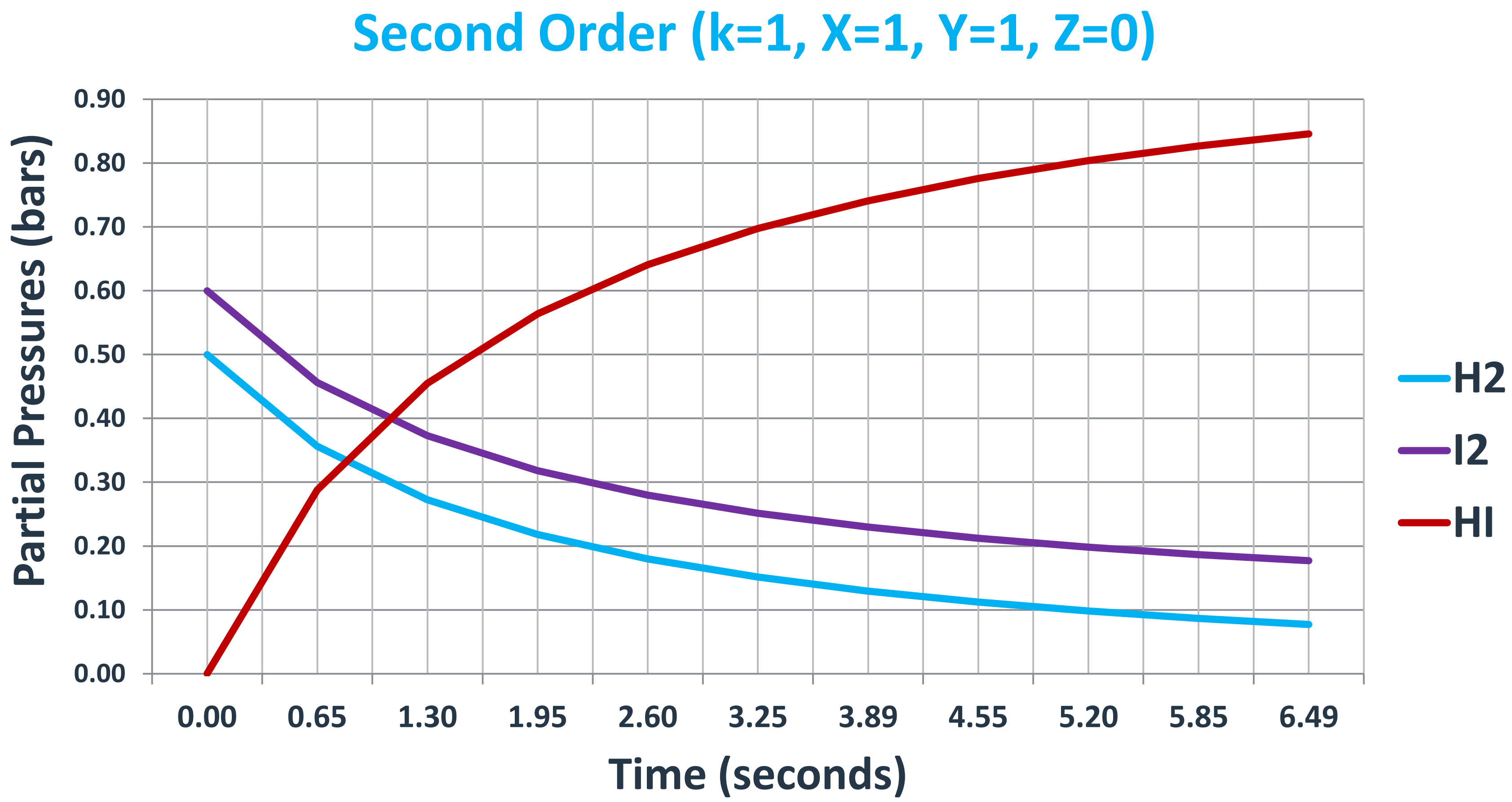
Kinetics

Effect of reaction order



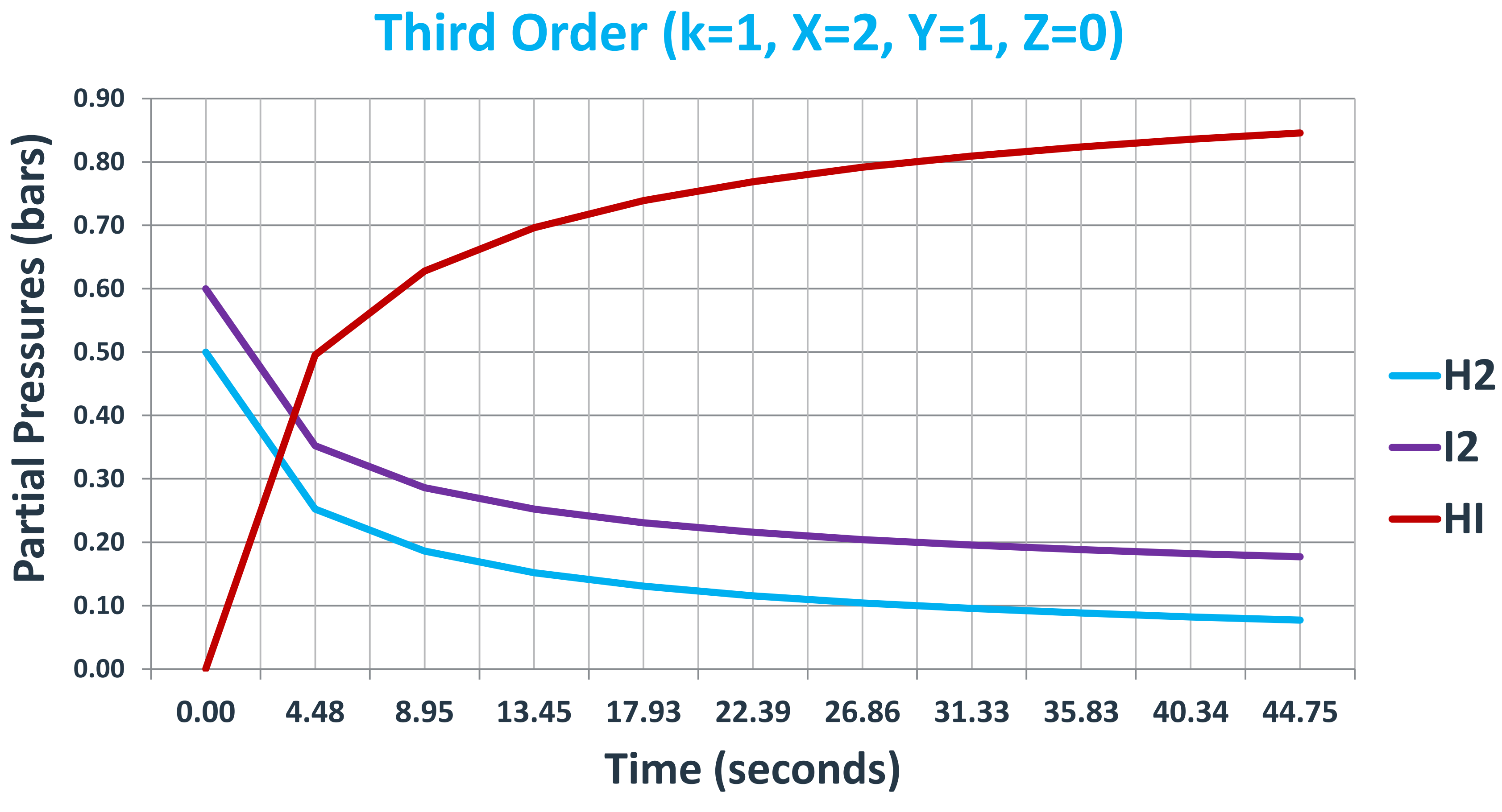
Kinetics

Effect of reaction order



Kinetics

Effect of reaction order



Kinetics
Effect of rate constant

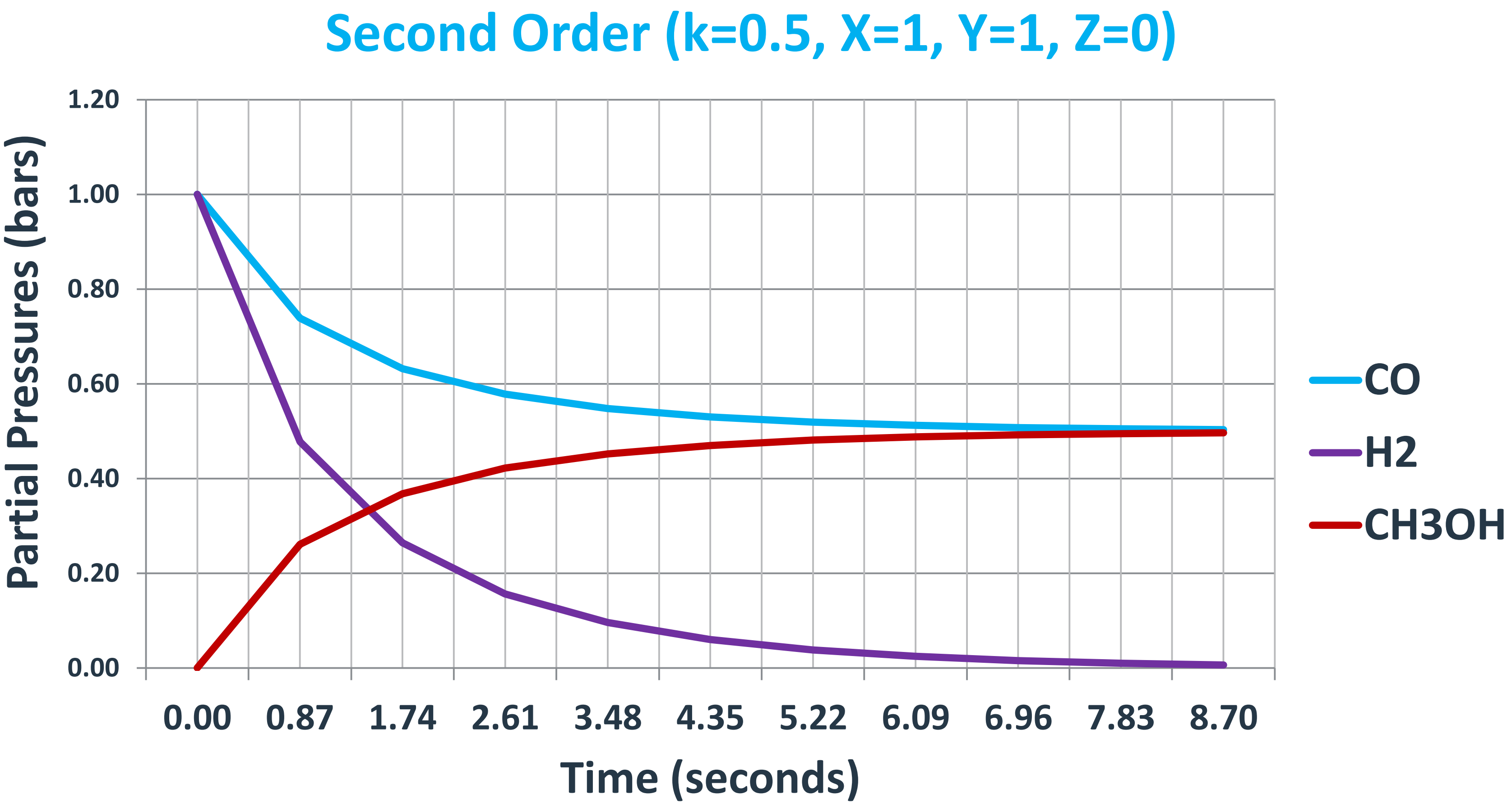
- **Reaction:**
  - **$CO\ (g) + 2H_2\ (g) \rightleftharpoons CH_3OH\ (g)$**
- **Virtual Experiment:**

ChemReaX

  - **Simulate a second-order reaction in ChemReaX , vary the rate constant, collect data**
    - Initial partial pressures: P(CO) = P(H2) = 1 bar; P(CH3OH) = 0
    - Temperature: 298.15K
  - **Plot the reaction progress vs. time**

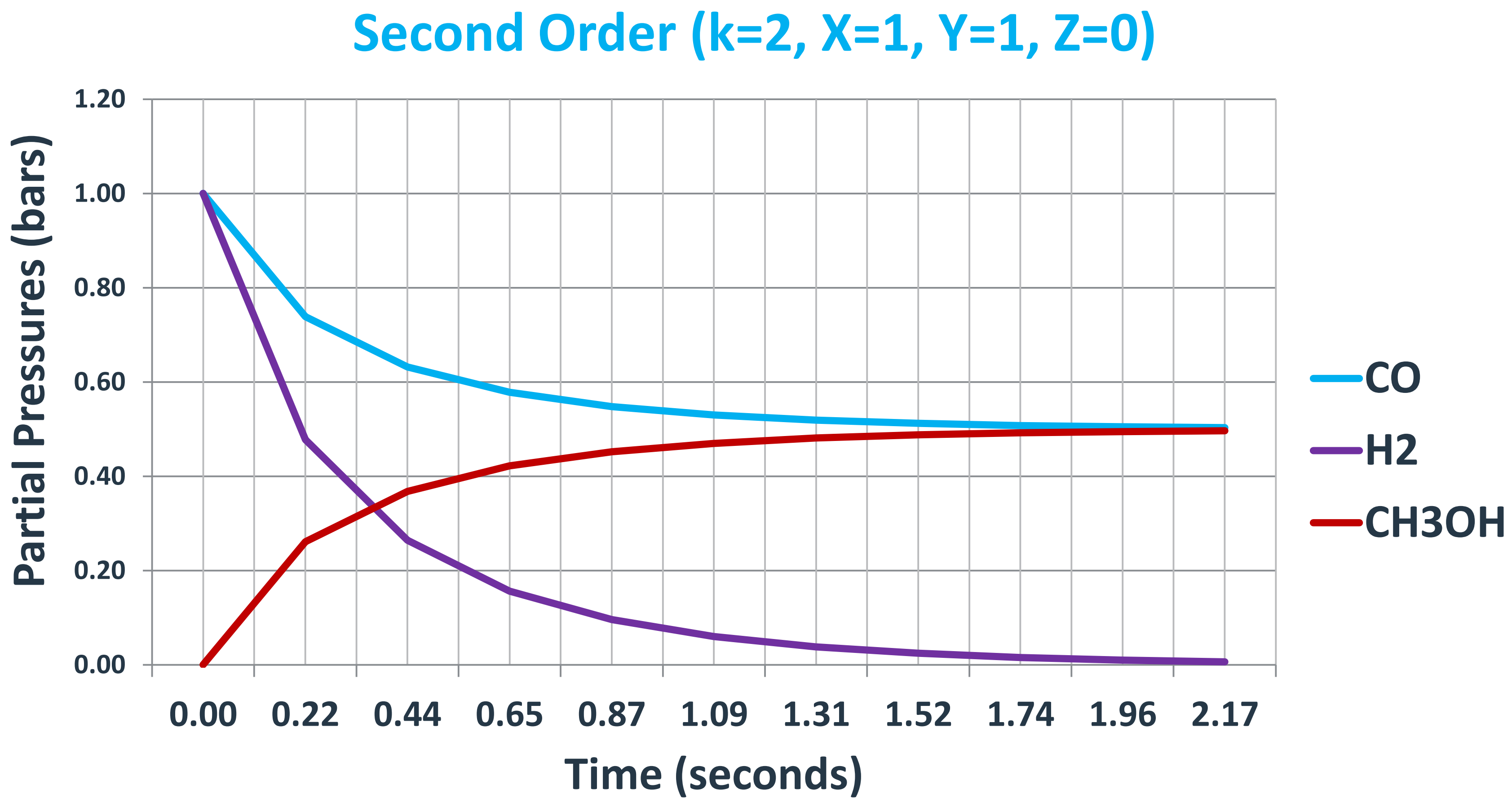
Kinetics

Effect of rate constant



Kinetics

Effect of rate constant



Kinetics

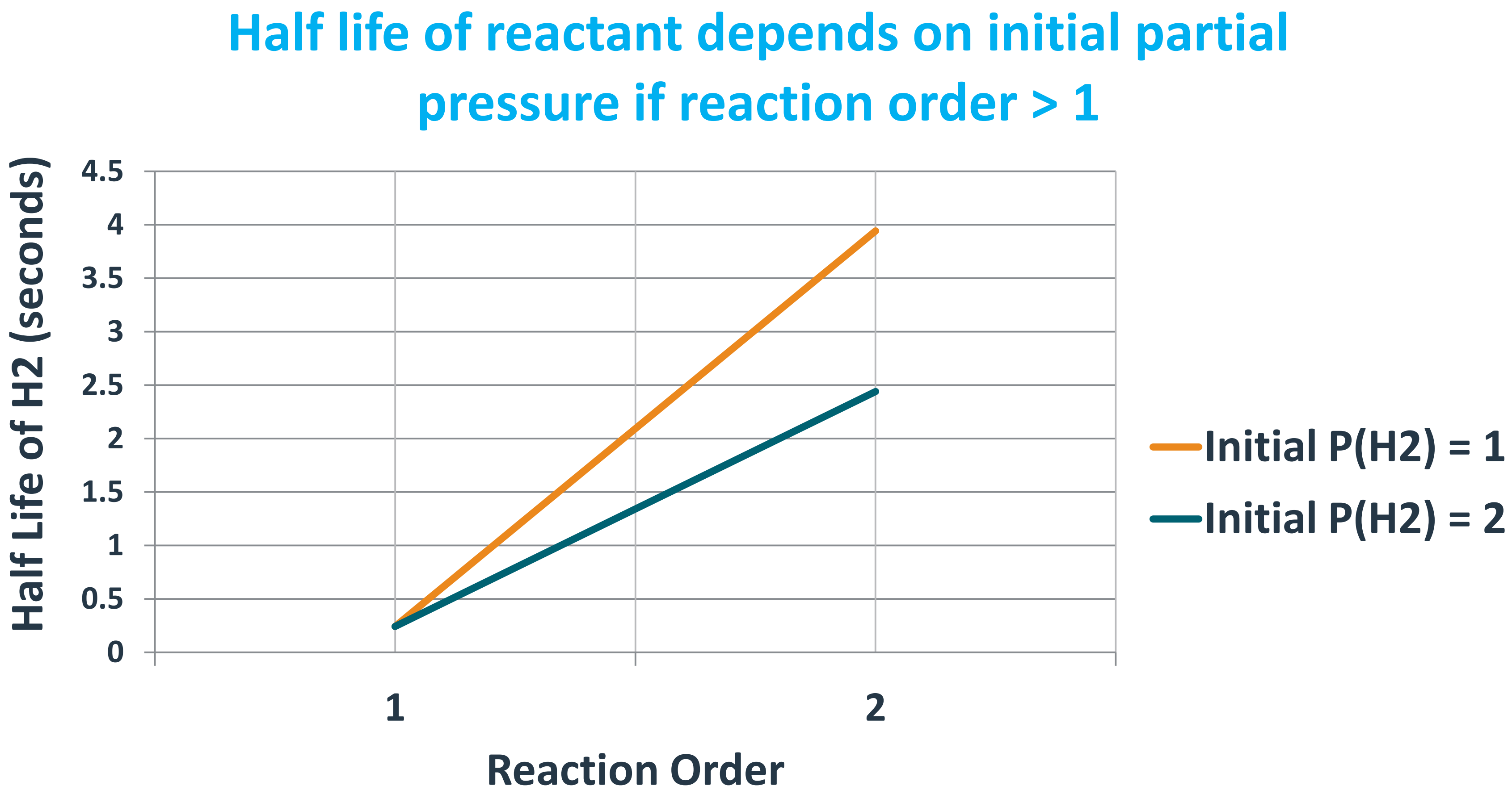
Half lives of reactants

- **Reaction:**
  - **$N_2 (g) + 3H_2 (g) \rightleftharpoons 2NH_3 (g)$**

- **Virtual Experiment:** ChemReaX
  - **Simulate as first and second order reactions, vary the initial partial pressure of H_2, and note the half lives of H_2**
    - Initial partial pressures: $P(N_2)$= 10 bar; $P(NH_3)$ = 0
    - Temperature: 298.15K
  - **Plot the half lives of H_2 vs. reaction order and initial partial pressure**

Kinetics

Half lives of reactants



Acid-Base Titration
Effect of Titrand Concentration

- **Reaction:**
  - **Titrand:** CH3CO2H**; Titrant:** NaOH
- **Virtual Experiment:**

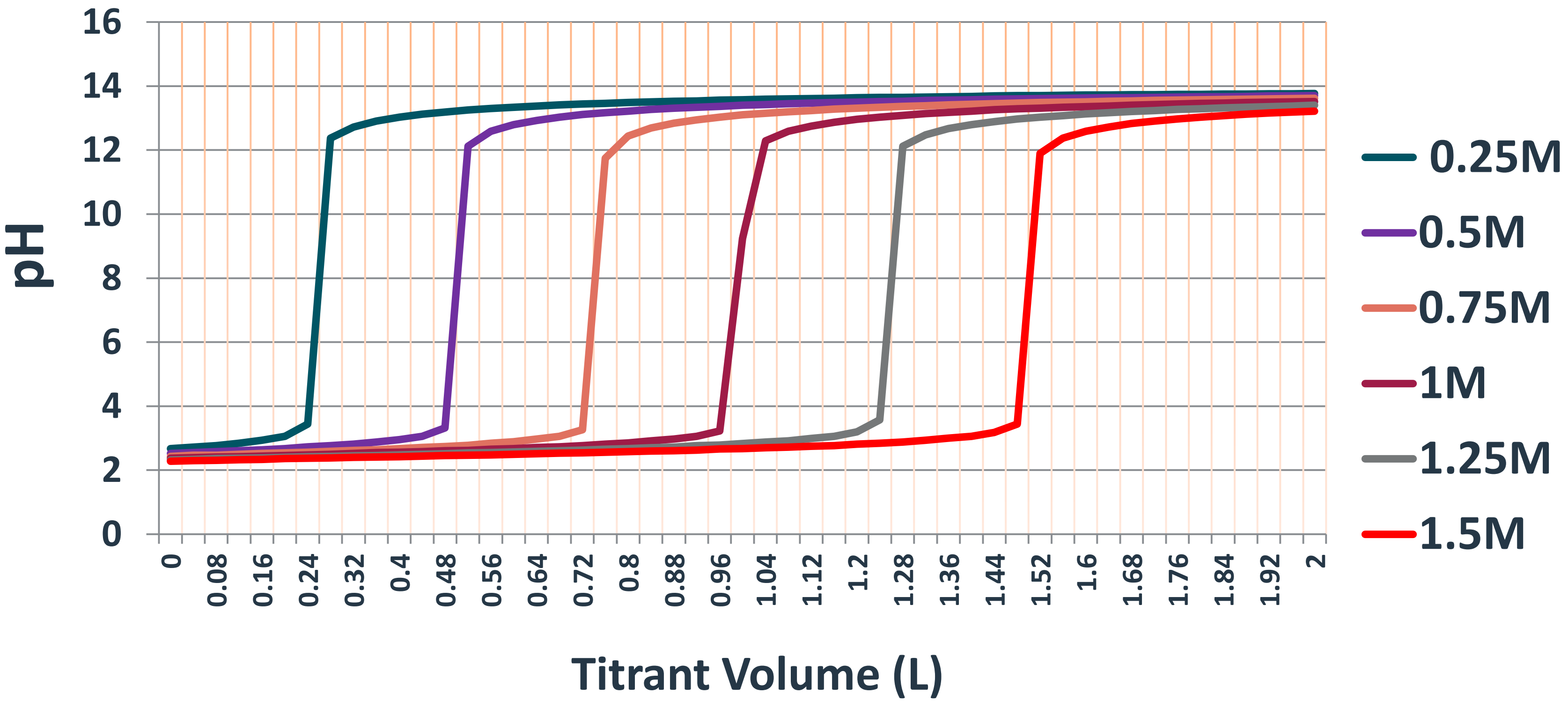
ChemReaX

  - **Run titration simulations in ChemReaX with varying titrand concentrations**
    - Titrand volume = 1L; Titrant concentration = 1M
  - **Plot the pH curves side-by-side**

Acid-Base Titration

Effect of Titrand Concentration

Equivalence point moves to the right as the titrand concentration increases



Acid-Base Titration

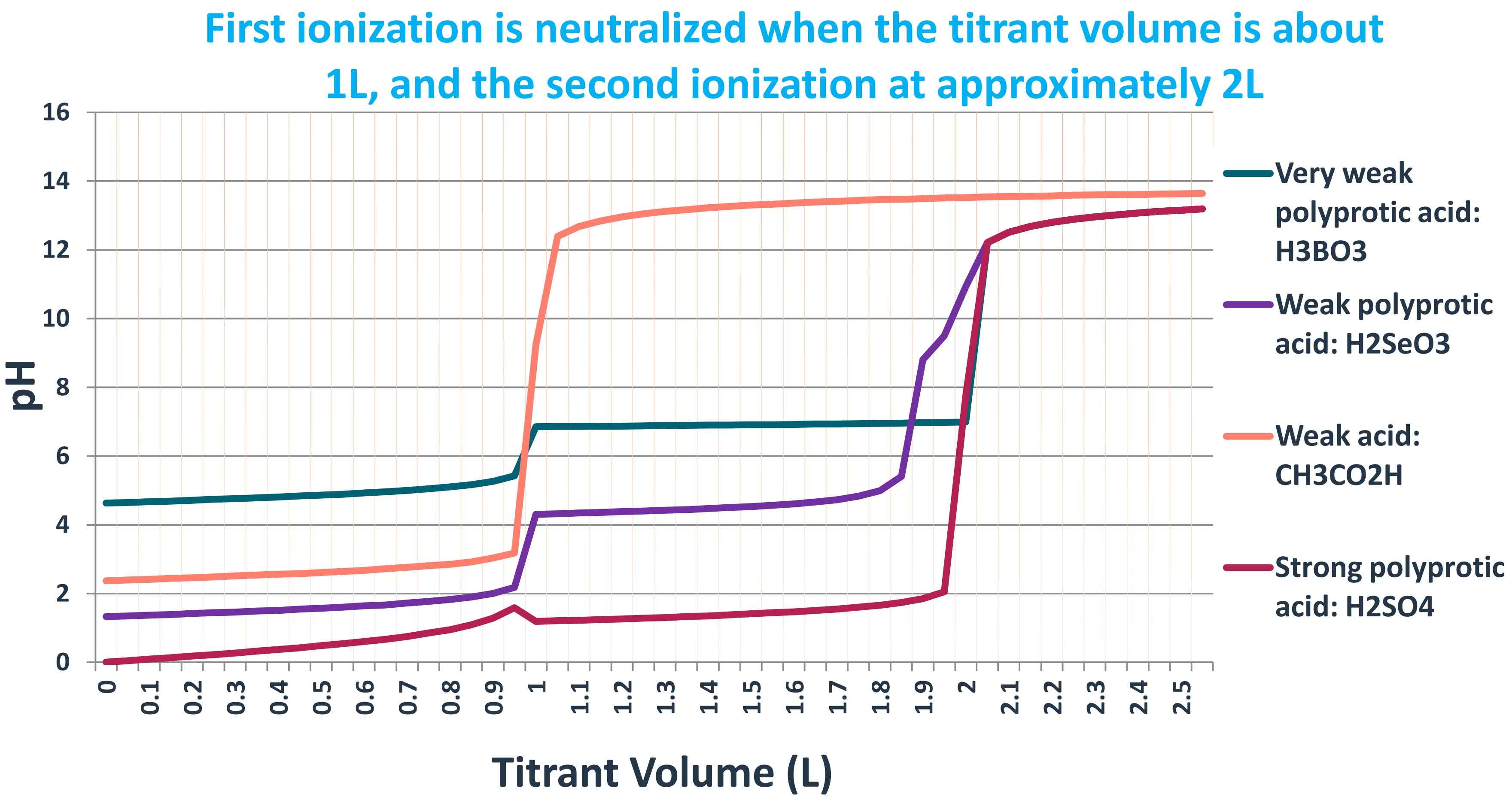
Comparing different acids

- **Reaction:**
  - **Titrands:** CH_3CO_2H, H_2SO_4, H_2SeO_3, H_3BO_3**; Titrant:** NaOH
- **Virtual Experiment:**

ChemReaX

  - **Run titration simulations of each titrand against the titrant using ChemReaX**
    - Titrand volume = 1L; Titrand/titrant concentrations = 1M
  - **Plot the pH curves side-by-side**

Acid-Base Titration
Comparing different acids



Acid-Base Titration

Effect of hydrolysis

- **Reaction:**
  - **Titrand:** H_2SeO_3**; Titrant:** NaOH
- **Virtual Experiment:**

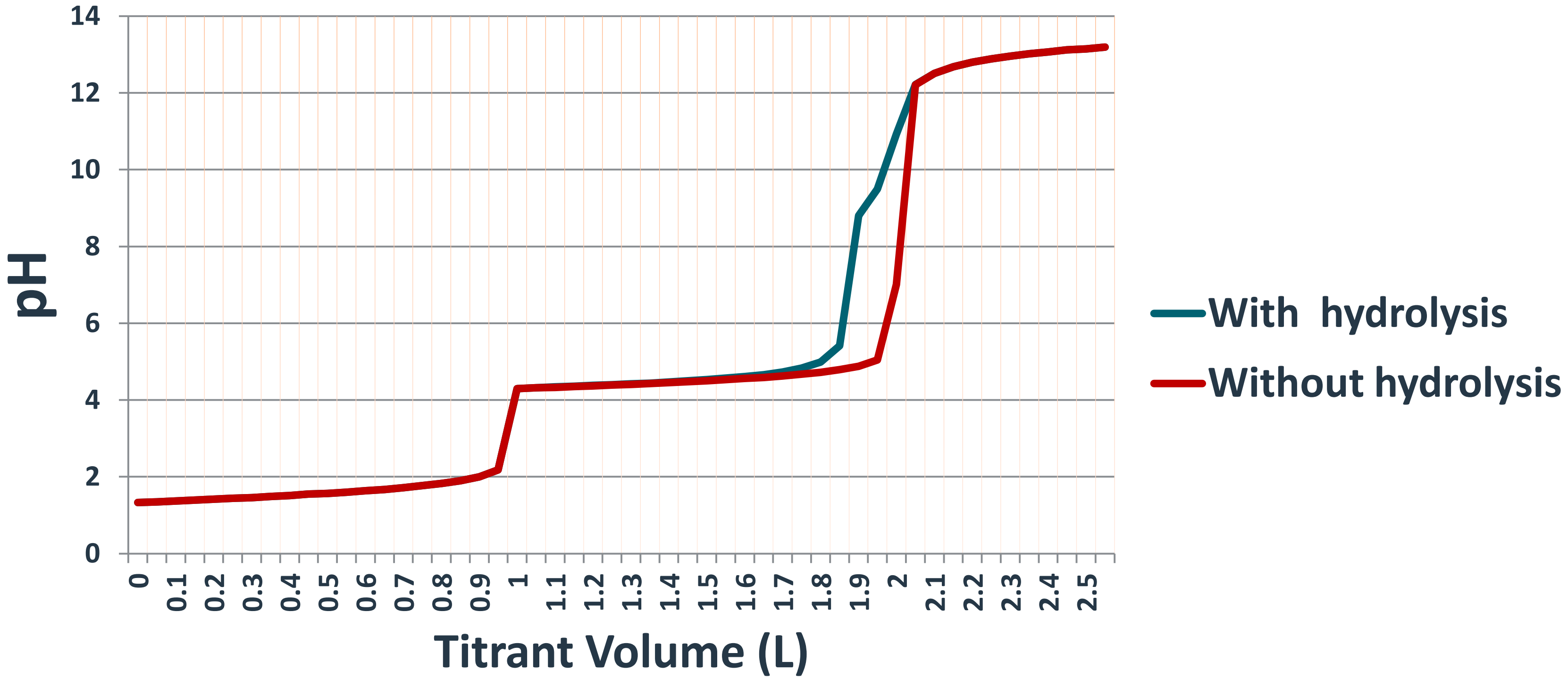
ChemReaX

  - **Run a titration simulation of titrand against the titrant using ChemReaX**
    - Titrand volume = 1L; Titrand/titrant concentrations = 1M
  - **Plot the pH curve with and without hydrolysis**

Acid-Base Titration

Effect of hydrolysis

Hydrolysis speeds up the neutralization of this polyprotic acid and accelerates the pH change



Gas Laws

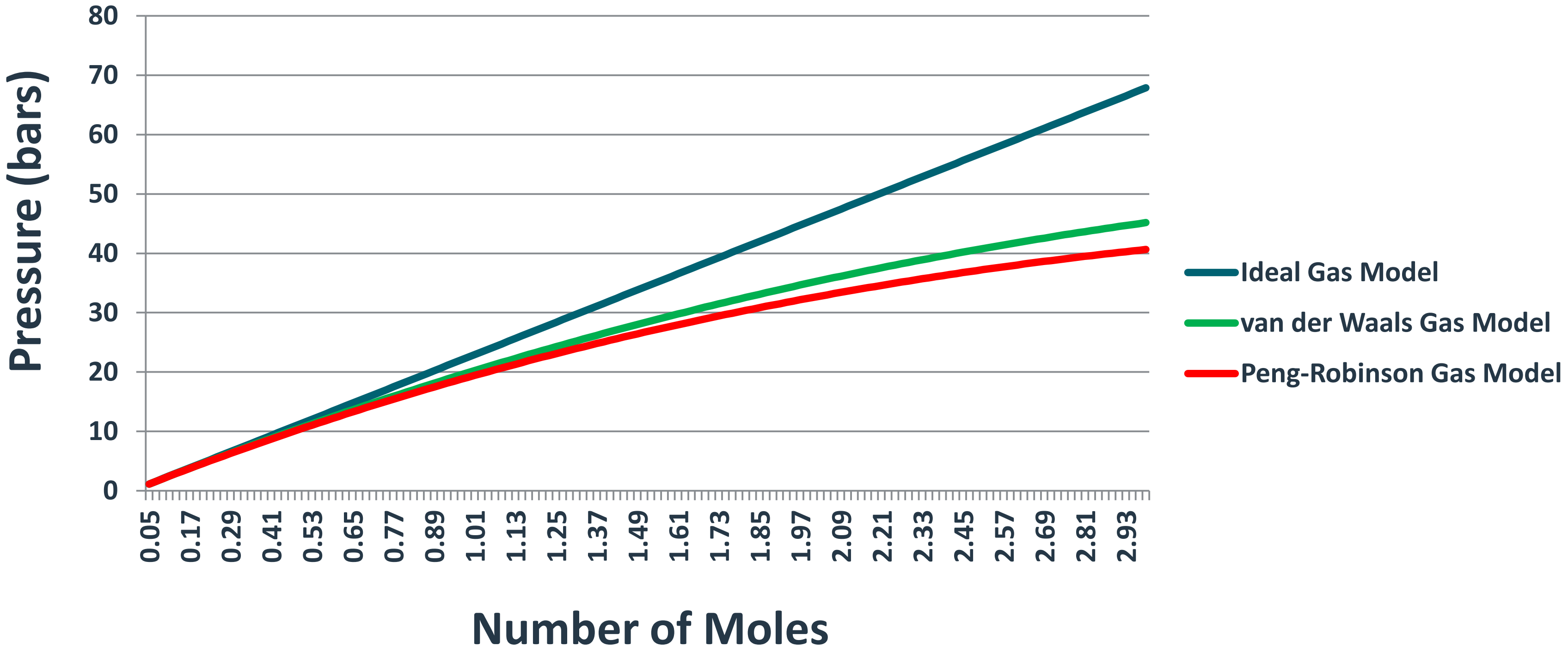
Deviation from the ideal gas law

- **Virtual Experiment:** [GasSim]
  - In a fixed volume of 1L, vary the number of moles of CO_2
  - Run GasSim simulations for temperatures below and well above the critical temperature T_c for CO_2 (304K)
  - Plot pressure vs. number of moles for the ideal gas law and " real" gas laws

Gas Laws

Deviation from the ideal gas law

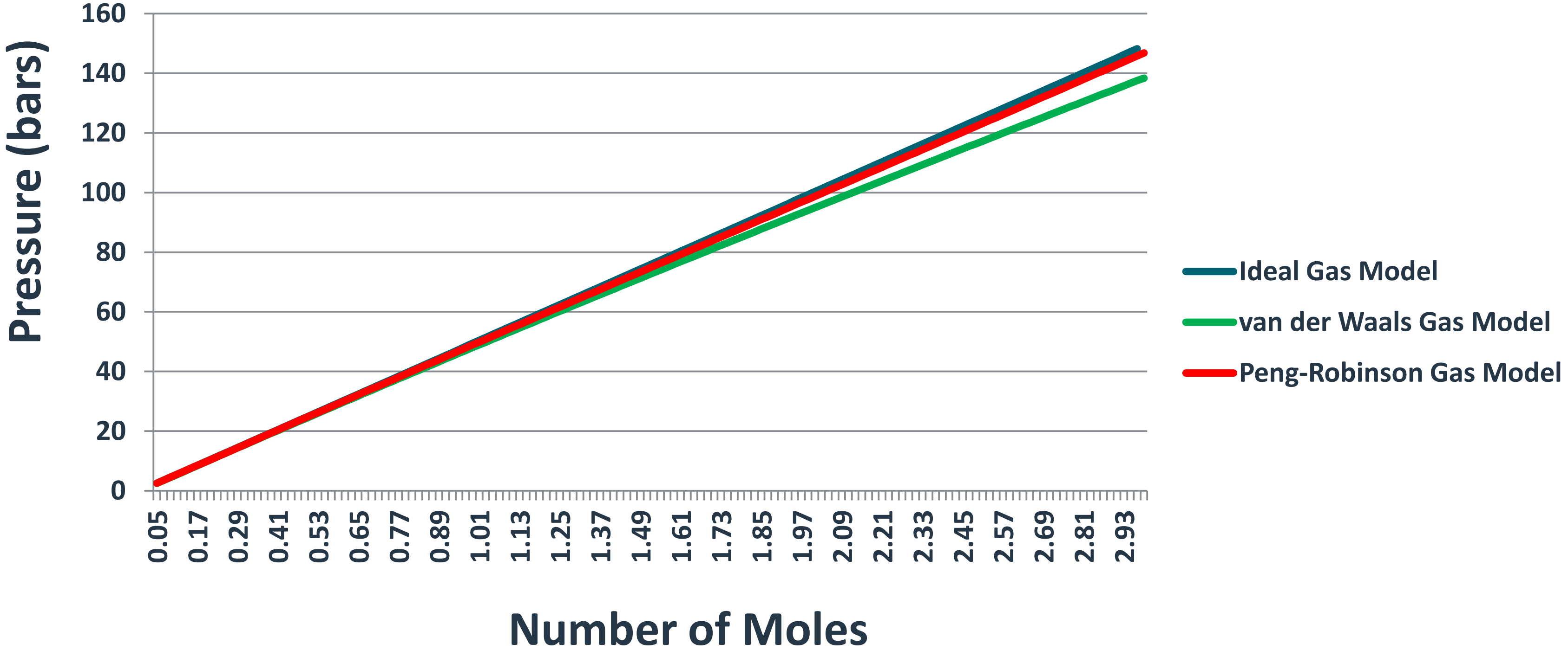
T = 273K < T_C: Inter-molecular attractive forces dominate at higher gas densities and reduce the pressure in "real" gas models



Gas Laws

Deviation from the ideal gas law

T = 600K > T_C: Both ideal and "real" gas models predict similar pressures -- inter-molecular attractive forces are mostly overcome by the higher kinetic energy



Why use virtual labs?

- Integrate demonstrations into lectures
- Supplement textbooks and real labs
- Bring textbook concepts to life
- Enable students to learn by doing
- Meet specific learning targets
- All at no cost to you or your students

Assigning and assessing virtual labs

- Can go beyond conventional lab reports
- Structure as quizzes in Google Forms:
  - guided sequence of experiments with questions to answer along the way
  - students run multiple simulations, collect data and perform additional calculations/analysis
  - students get quick feedback and scores
  - assign in-class or as homework
- Sample exercises: www.sciencebysimulation.com/chemreax/Exercises.aspx

Feedback? Questions? Need help?

Please email us at:

info@sciencebysimulation.com