Cubic Equation of State

Talk to a Teacher
http://spoken-tutorial.org
National Mission on Education through ICT
http://sakshat.ac.in

Priya Bagde
IIT Bombay

15 June 2013

Learning Objectives

We will learn how to

- **Create a reusable model**
- **Reuse the model for different components**
- **Import data from Thermodynamics library**
- **Solve the model**

System Requirements

System Requirements

- **Ubuntu Linux OS v.12.04**

System Requirements

- **Ubuntu Linux OS v.12.04**
- **ASCEND v.0.9.8**

User must have basic knowledge of

Pre-requisites

User must have basic knowledge of

- **Linux**
- **ASCEND**
- **Peng Robinson cubic EOS**

To know more about ASCEND,

To know more about ASCEND,

- **Please visit ascend4.org**

To know more about ASCEND,

- **Please visit ascend4.org**
- **For relevant tutorials, please visit http://spoken-tutorial.org**

Peng Robinson Cubic EOS

$$p = \frac{\bar{R}T}{\bar{v} - b} - \frac{a(T)}{\bar{v}(\bar{v} + b) + b(\bar{v} - b)}$$

where

$$a(T) = 0.45724 \frac{\bar{R}^2 T_c^{\,2}}{p_c} \alpha(T)$$

$$\alpha = \left(1 + \kappa \left(1 - \sqrt{\frac{T}{T_c}}\right)\right)^2$$

$$\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

$$b = \frac{0.0778 \bar{R} T_c}{p_c}$$

Peng Robinson Cubic EOS

It is sometime more convenient to express the equation as a polynomial in terms of compressibilty factor Z

$$Z^3 + (-1 + B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0$$

in which

$$A = \frac{a(T)p}{(\bar{R}T)^2}$$

$$B = \frac{bp}{\bar{R}T}$$

$$Z = \frac{p\bar{v}}{\bar{R}T}$$

Summary

We have learnt how to

- **create a reusable model**
- **Reuse the model for different components**
- **Import data from the Thermodynamics library**
- **solve the model**

Assignment

- **Modify pengrobinson model to solve the value of V**
- **Reuse this model in a test model**
- **Compute value of V for a Ethylene**

About the Spoken Tutorial Project

- **Watch the video available at http://spoken-tutorial.org /What_is_a_Spoken_Tutorial**

- **It summarizes the Spoken Tutorial project**

About the Spoken Tutorial Project

- Watch the video available at
  http://spoken-tutorial.org
  /What_is_a_Spoken_Tutorial
- It summarizes the Spoken Tutorial project
- If you do not have good bandwidth, you can download and watch it

Spoken Tutorial Workshops

The Spoken Tutorial Project Team

- ▶ **Conducts workshops using spoken tutorials**
- ▶ **Gives certificates to those who pass an online test**
- ▶ **For more details, please write to contact@spoken-tutorial.org**

Acknowledgments

- **Spoken Tutorial Project is a part of the Talk to a Teacher project**
- **It is supported by the National Mission on Education through ICT, MHRD, Government of India**
- **More information on this Mission is available at http://spoken-tutorial.org /NMEICT-Intro**