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ANTOINE CONSTANT PARAMETRS PREDICTION BY USING GAMS(GENERAL ALGEBRAIC MODELING SYSTEM)

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Abstract : Antoine constants are fundamental parameters used to calculate vapor pressure of pure substances, essential in the design and simulation of separation processes. Although experimental Antoine constants are widely reported for many chemicals, they are often unavailable for newly synthesized or less common compounds. This research explores methods for predicting Antoine constants using GAMS regression-based approaches.*This is useful to predict accurate vapor pressure estimation is feasible when experimental data is lacking*.

IndexTerms - **antoine constant,GAMS, vapor pressure,design**

I. INTRODUCTION

The Antoine constants are empirical, derived by curve-fitting experimental vapor-pressure vs temperature data over specified ranges—accuracy drops outside those bounds. Different sources (e.g. **Perry's Handbook**, **Poling et al.**, **Yaws & Yang**) publish slightly varying values because of differences in fitting methodology and temperature range assumptions. For instance, one source gives water as A = 16.3872, B = 3885.70, C = 230.170 valid from 0–200 °C.

GAMS (General Algebraic Modeling System) is a high-level modeling system for mathematical programming problems. It is designed for building and solving large-scale optimization problems, such as:

- Linear Programming (LP)
- Mixed Integer Programming (MIP)
- Nonlinear Programming (NLP)
- Mixed Integer Nonlinear Programming (MINLP)
- Dynamic systems and equilibrium models

1. METHOD:

ANTOINE EQUATION:

The Antoine equation is an empirical relationship that describes vapor pressure as a function of temperature. Its constants are determined from experimental data and are

valid only within a specific range of temperatures and pressures.

$$\ln P^{sat} = A - \left(\frac{B}{T+C}\right) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

Where, P = Vapor pressure in kPa

T = Temperature, K

A, B, C = Antoine Constant.

3. Pure Component Modelling

Pure component P-T data literature was regressed to obtain the Antoine Constant using GAMS.

Vapour Pressure data are requires for design of chemical engineering equipment. In **chemical engineering**, **Antoine constants** are widely used for calculating **vapor pressure**, which is critical in many core processes

3.1 Applucations of Chemical Engineering.

1, Distillation Design

Antoine constants are used to calculate vapor-liquid equilibrium (VLE), essential for sizing and modeling distillation columns.

2, Flash & Evaporation Calculations

Vapor pressure is required to determine how much of a component vaporizes at a given pressure/temperature.

2. **Boiling Point Estimation**
   Helps find the **boiling point** of a substance at any pressure, or vice versa.
3. **Reactor Design**

In reactions involving volatile components, accurate vapor pressure prediction is needed for pressure control and safety.

4. Environmental Engineering
   Used to estimate VOC emissions or component losses by evaporation
5. Heat Exchanger Design
   Knowing when a fluid will boil or condense helps size and design **condensers and reboilers**.
6. Safety & Relief Valve Design
   Required for predicting pressures at various temperatures in case of runaway reactions or overheating.

4. PROCEDURE

The experimental data from literature was taken for the component water and the regression was done uisn GAMS programming

The steps for predicting antoine constant is mentioned below:

Step 1: Prepare Experimental Data
You'll need a set of known vapor pressure and temperature data.
Step 2: Define Sets and Parameters in GAMS
Step 3: Declare Variables
Step 4: Define Equations
Step 5: Set Initial Values and Bounds
Step 6: Solve the Model

The estimated values of A, B, and C for the given compound based on the best fit to the experimental data.

5.RESULTS AND DISCUSSIONS

The Antoine Constant predicted by GAMS

A= 10.307

B=3455.945 & C = 365.468

The sum of squared error is reported to be 2.63×10^{-4} which is very much acceptable

The literature value for Antoine Constant for water [1] is A=8.07131 ,B=1730.63 and C=233.426

NOMENCLATURE

P Total Pressure,Pa
T Absolute Temperature,K
R Universal Gas Constant,J K-1mol-1

CONCLUSION

The study confirms that Antoine constants can be reliably estimated using GAMS

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