State Conditions Transferability Problem

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The Third Industrial Fluid Properties Simulation Challenge
http://fluidproperties.org/

Computational Molecular Science and Engineering Forum

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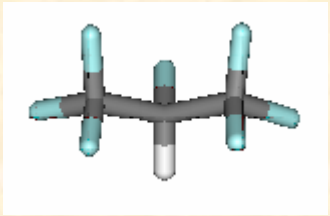
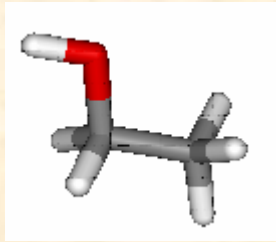
Problem Statement

- **For the binary system...**
  1,1,1,2,3,3,3-heptafluoropropane (HFC-227ea) and ethanol





- **... compute bubble point pressures for 7 different compositions at constant temperature (343 K).**

- **Given are experimentally determined isothermal bubble point pressures for 13 different mixture compositions (283 K.)**
- **Furthermore, given are pure component vapor pressures for both temperatures.**

Problem Motivation

- **Extrapolation from an experimentally known state condition to an unknown can be very difficult for certain properties.**

- **A few methods for that kind of problem have been developed for pure component properties**
  - **for example the method by Pailhes uses a single low pressure boiling point to estimate the normal boiling point**

- **BUT most industrial systems are mixtures!**
- **There is a lack of methods for that kind of problem for fluid mixture properties, like VLE, LLE, etc.**
- **Standard models in process engineering, like g^E-models or cubic equations-of-state, typically do not perform well for this kind of task.**

Contest Rules

- **The force field employed must be capable of describing the interactions of each of the molecules in a consistent manner.**
  - **The same force field must be used in all calculations.**
- **Any force field previously published in the open literature prior to the announcement of this challenge is acceptable, as long as its development adheres to the condition above.**
- **There is no limitation on the experimental data for the individual components that can be used to parameterize a model.**
- **No mixture data (binary and/or higher order) for the specified system can be used other than the experimental data provided as part of the problem description.**
- **Estimates of uncertainty for computed bubble point pressure must be included.**
- **Any theory/modeling/simulation method, e.g. group contribution methods, can be used provided that the above rules are followed with respect to parameterization and application.**

Contest Scoring

- **Scoring was done by using the following simple formula**

$$F = \frac{100}{7} * \sum_{i=1}^{7} \left| \frac{P_{i,\exp} - P_{i,calc}}{P_{i,\exp}} \right|$$

- **where $P_{i,exp}$ and $P_{i,calc}$ are experimental and calculated bubble point pressures respectively for the mixture of composition *i*.**
  - **The pure component vapor pressures do not count for the scoring, since they are provided as input for model development.**

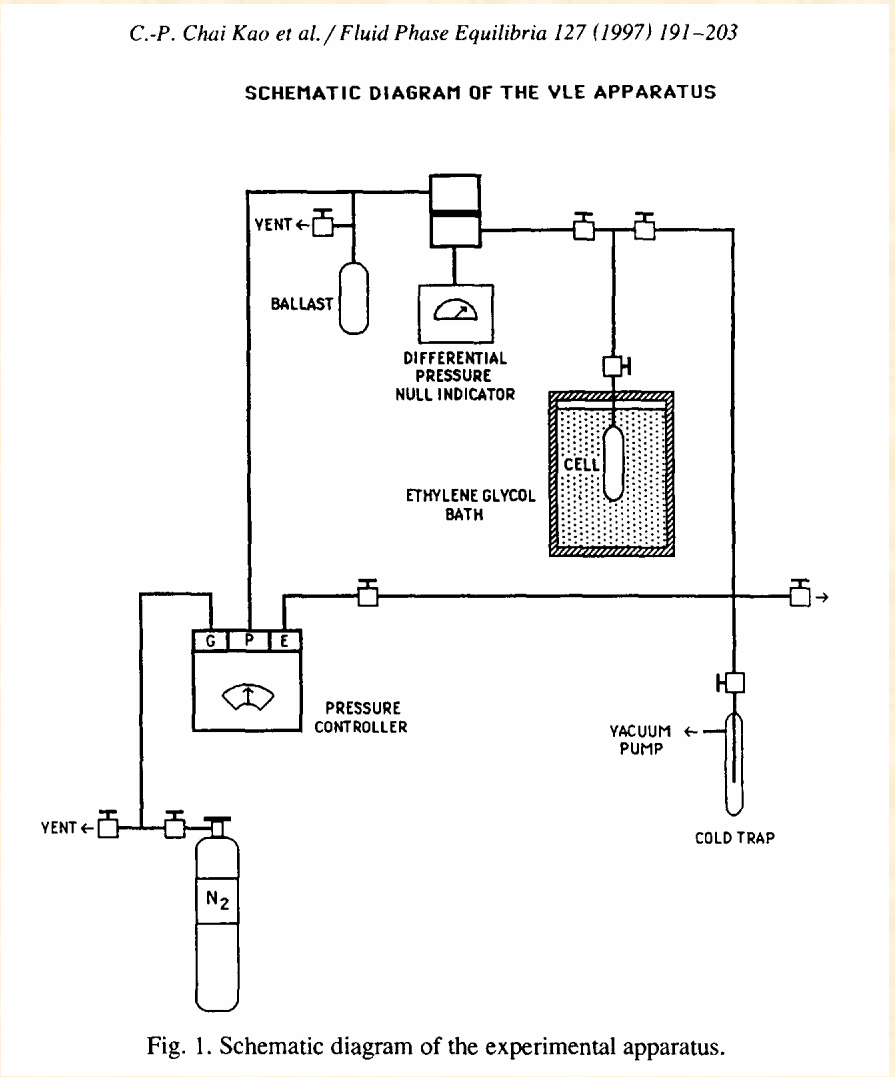
- **The entry with the lowest score F wins the competition.**

Nine Entries (Alphabetical Order)

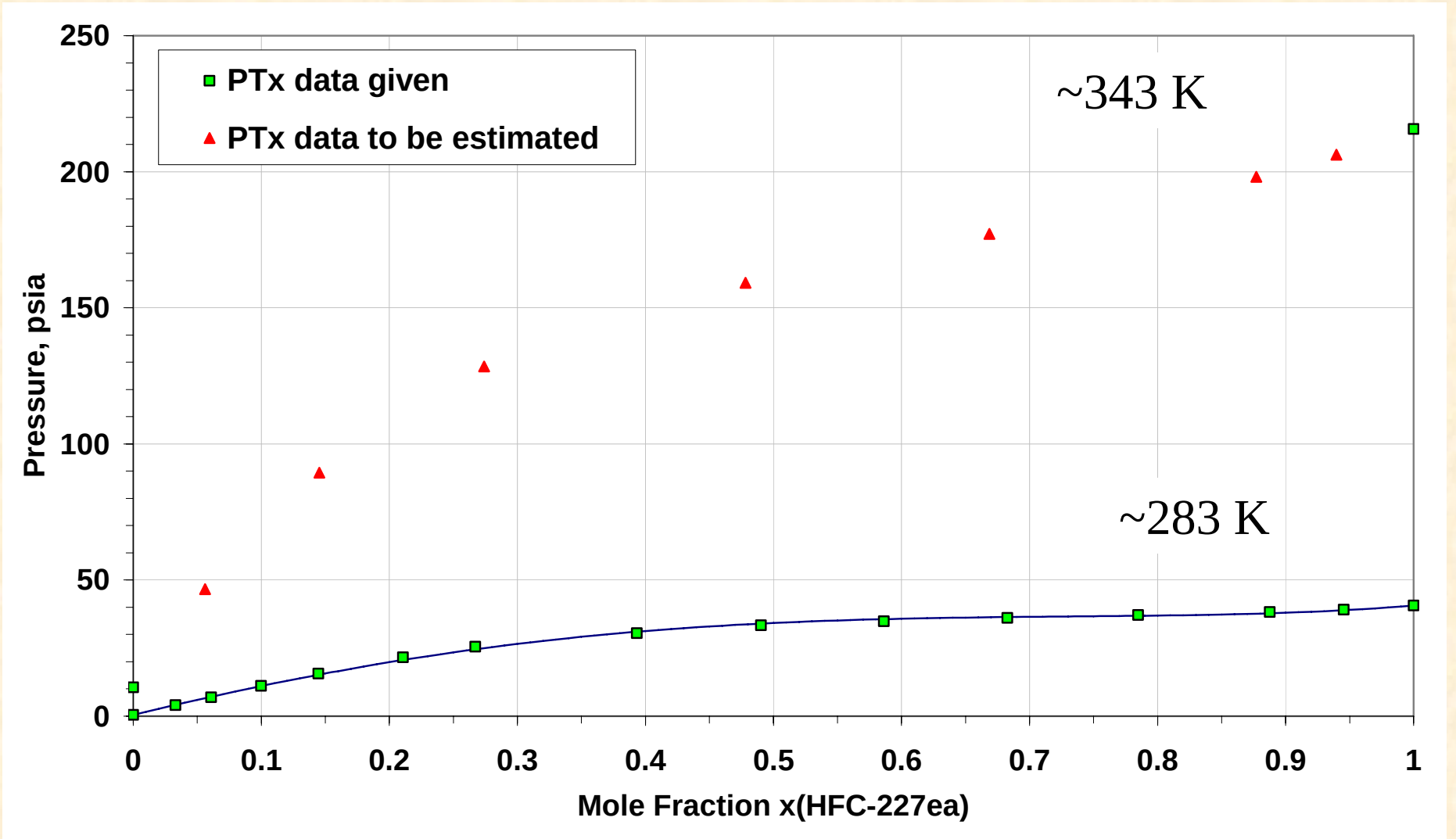
- **Christensen S., Peters G.H., Hansen F.Y., O'Connell J.P. and Abildskov J.**
  - **Technical University of Denmark, Lyngby**
- **Eckl B., Huang Y.-L., Vrabec J. and Hasse H.**
  - **University of Stuttgart , Germany**
- **Klamt A. and Eckert F.**
  - **COSMOlogic, Germany**
- **Kleiner M. and Sadowski G.**
  - **University of Dortmund, Germany**
- **Li X., Dai J., and Sun H.**
  - **Shanghai Jiao Tong University, China**
- **Rai N., Rafferty J.L. and Siepmann J.I.**
  - **University of Minnesota, Minneapolis, USA**
- **Rogankov V.B. and Byutner O.G.**
  - **Odessa State Academy of Refrigeration, Ukraine**
- **Sans A.D. and Elliott J.R.**
  - **The University of Akron, Akron Ohio, USA**
- **Yazaydin A.O. and Martin M.G.**
  - **Sandia National Laboratories, Albuquerque, USA**

VLE – Experimental Measurement

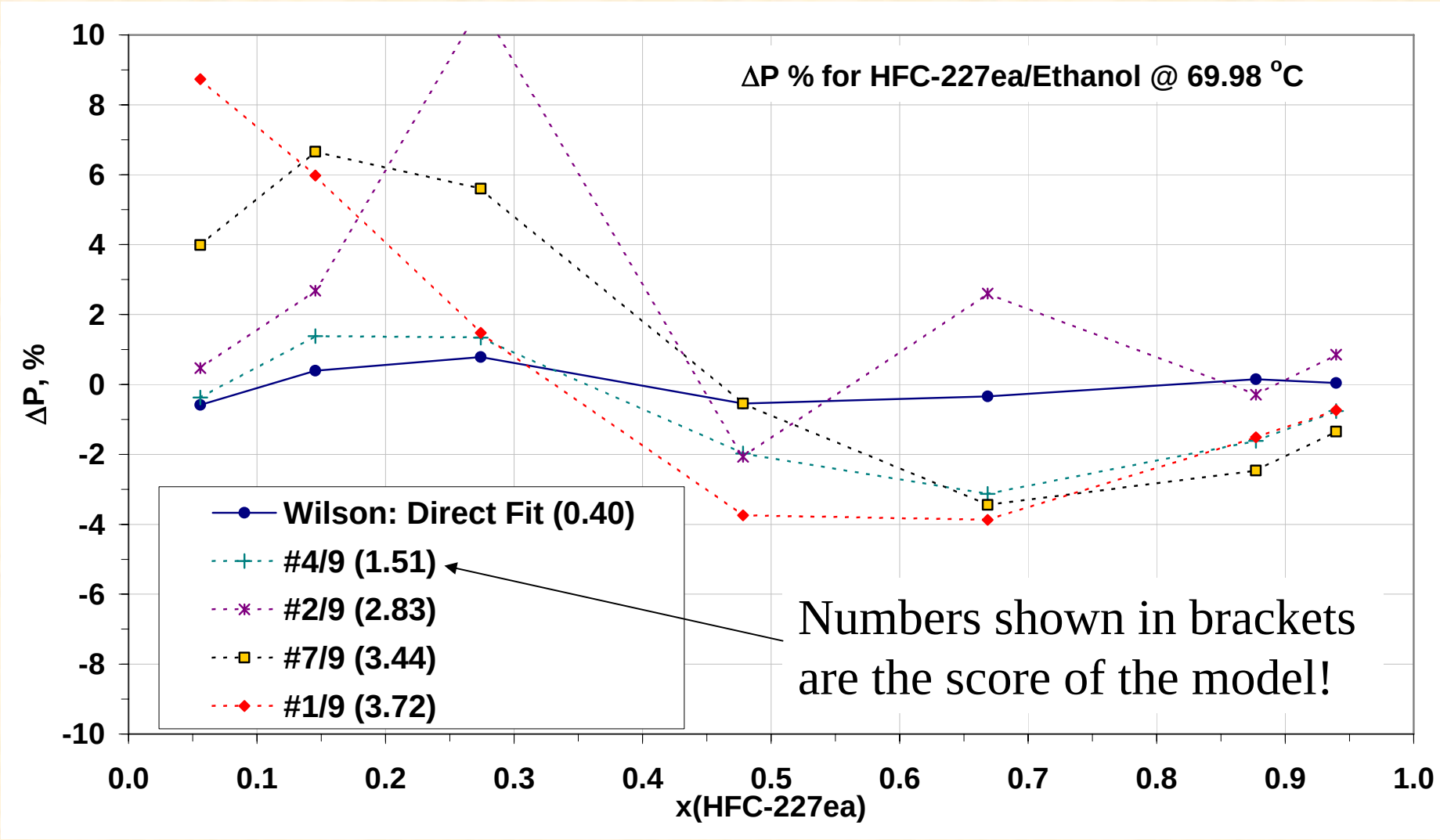
- **Data measured by C.-P. Chai Kao, DuPont**
- **Static apparatus**
  - **Kao et al., Fluid Phase Equilibria Vol. 127, 191(1997)**
- **Estimated uncertainty: Bubble point pressures to within +/- 0.2% for all points measured**



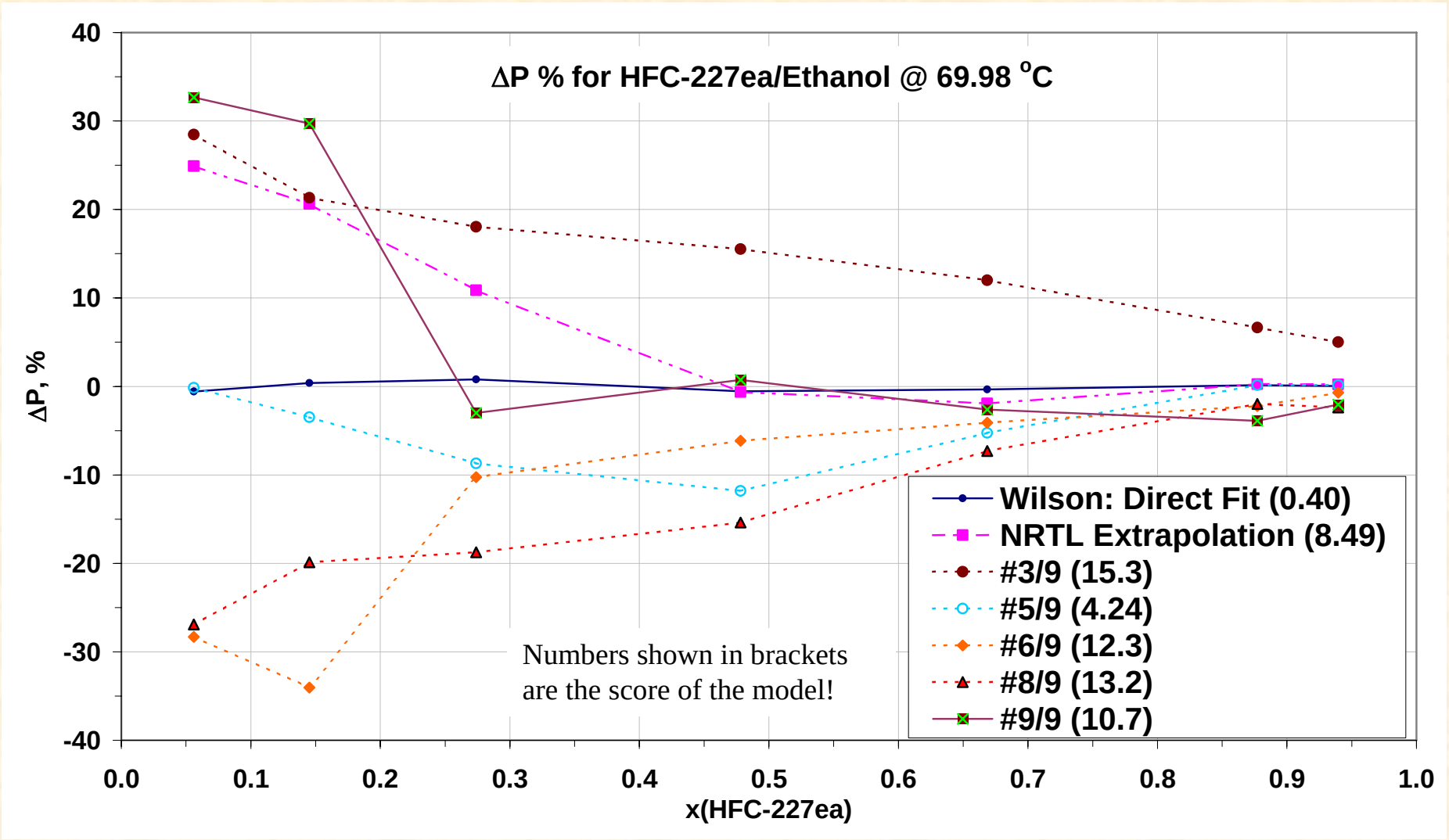
Bubble Point Pressure HFC-227ea/Ethanol



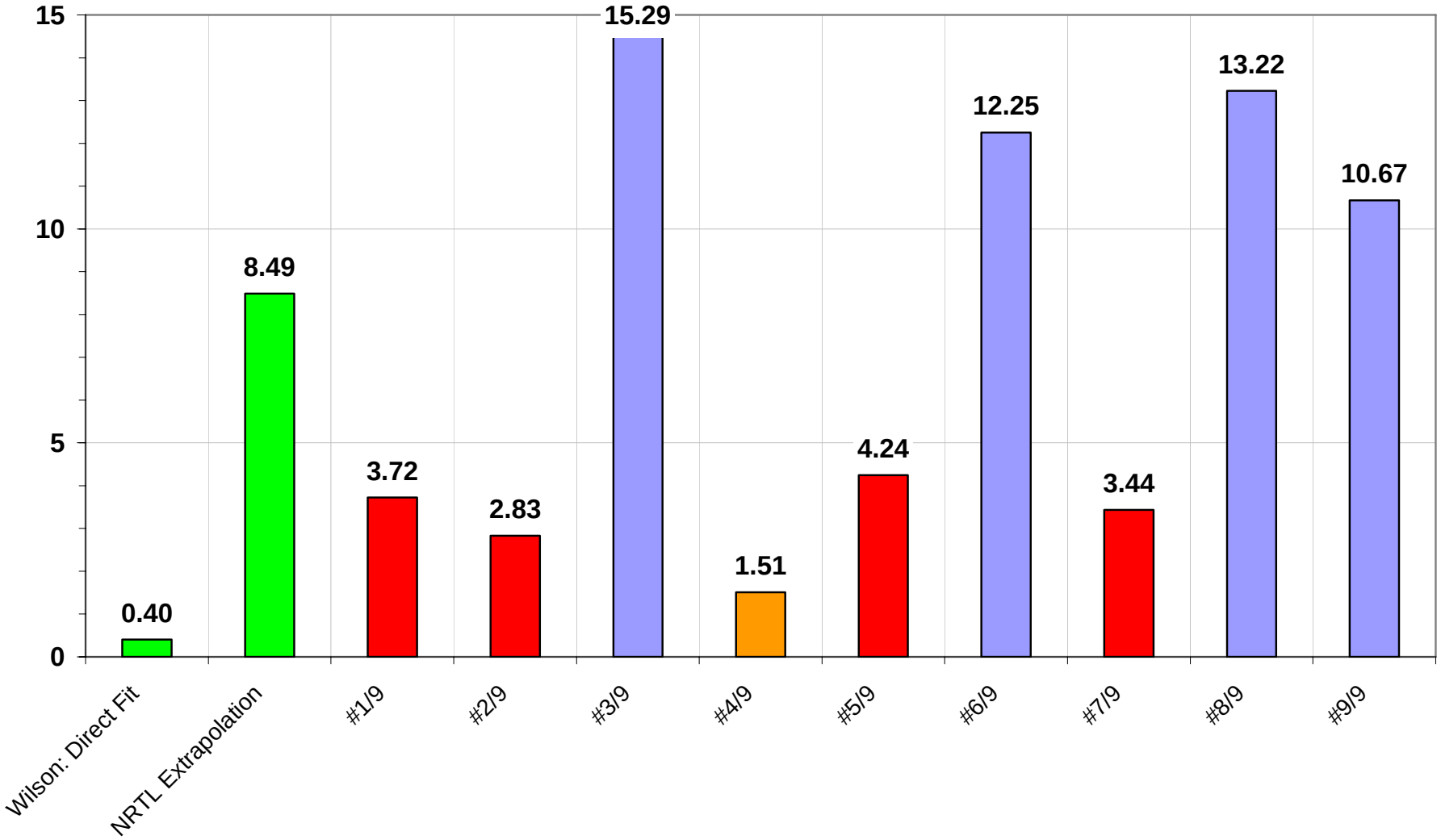
Quantitative Comparisons Part I



Quantitative Comparisons Part II



Quantitative Comparisons Part III



The Winner Is...

- **S. Christensen, G.H. Peters, F.Y. Hansen, J.P. O'Connell and J. Abildskov**
  - **Technical University of Denmark, Lyngby**

Runners up:

- **B. Eckl, Y.-L. Huang, J. Vrabec and H. Hasse**
  - **University of Stuttgart , Germany**
- **A. Klamt and F. Eckert**
  - **COSMOlogic, Germany**
- **M. Kleiner and G. Sadowski**
  - **University of Dortmund, Germany**
- **N. Rai, J. L. Rafferty and J. I. Siepmann**
  - **University of Minnesota, USA**