University of KwaZulu Natal
Chemical Engineering

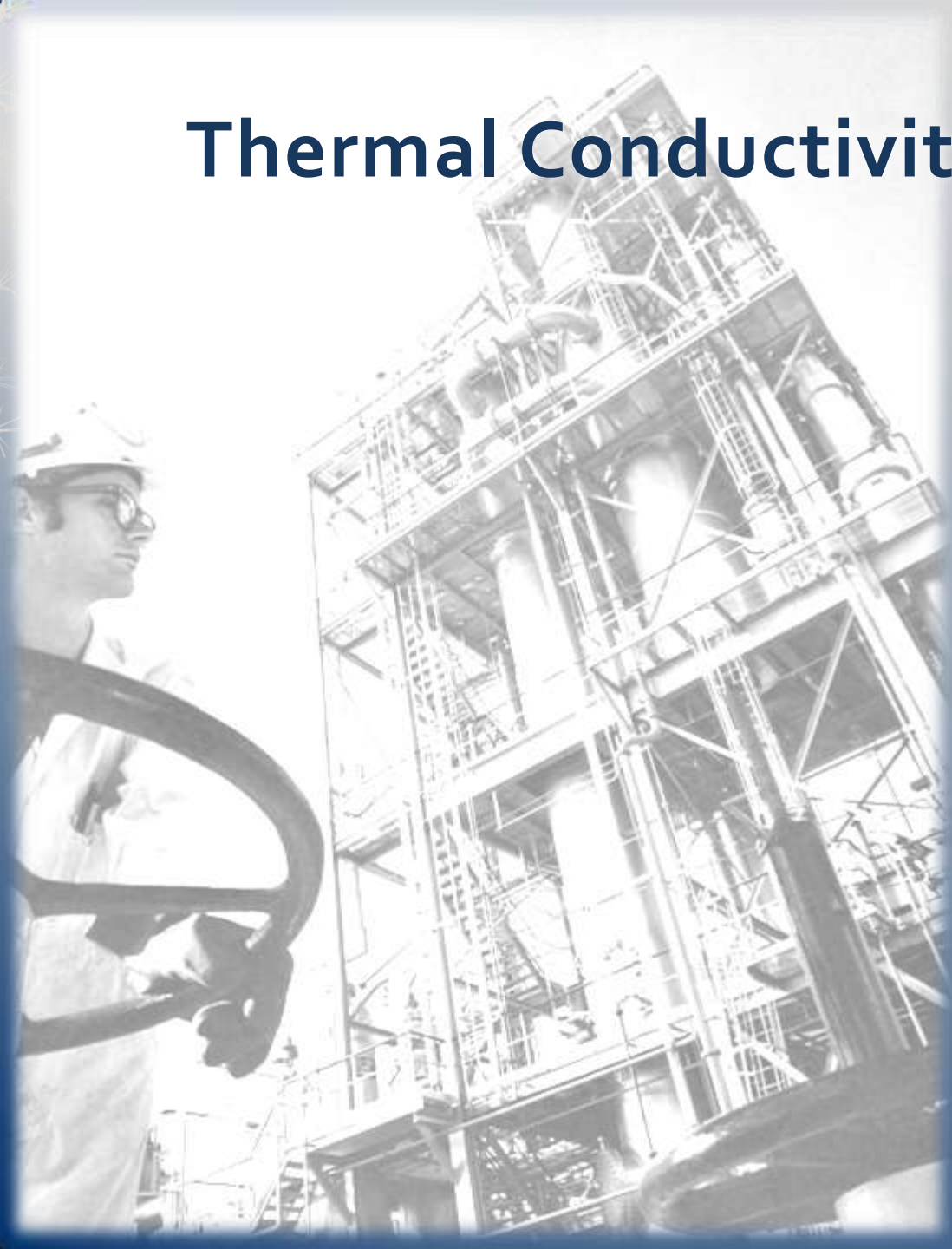
# A New Group Contribution Method For The Estimation Of Thermal Conductivity For Non-Electrolyte Organic Compounds

Onellan Govender

205502080

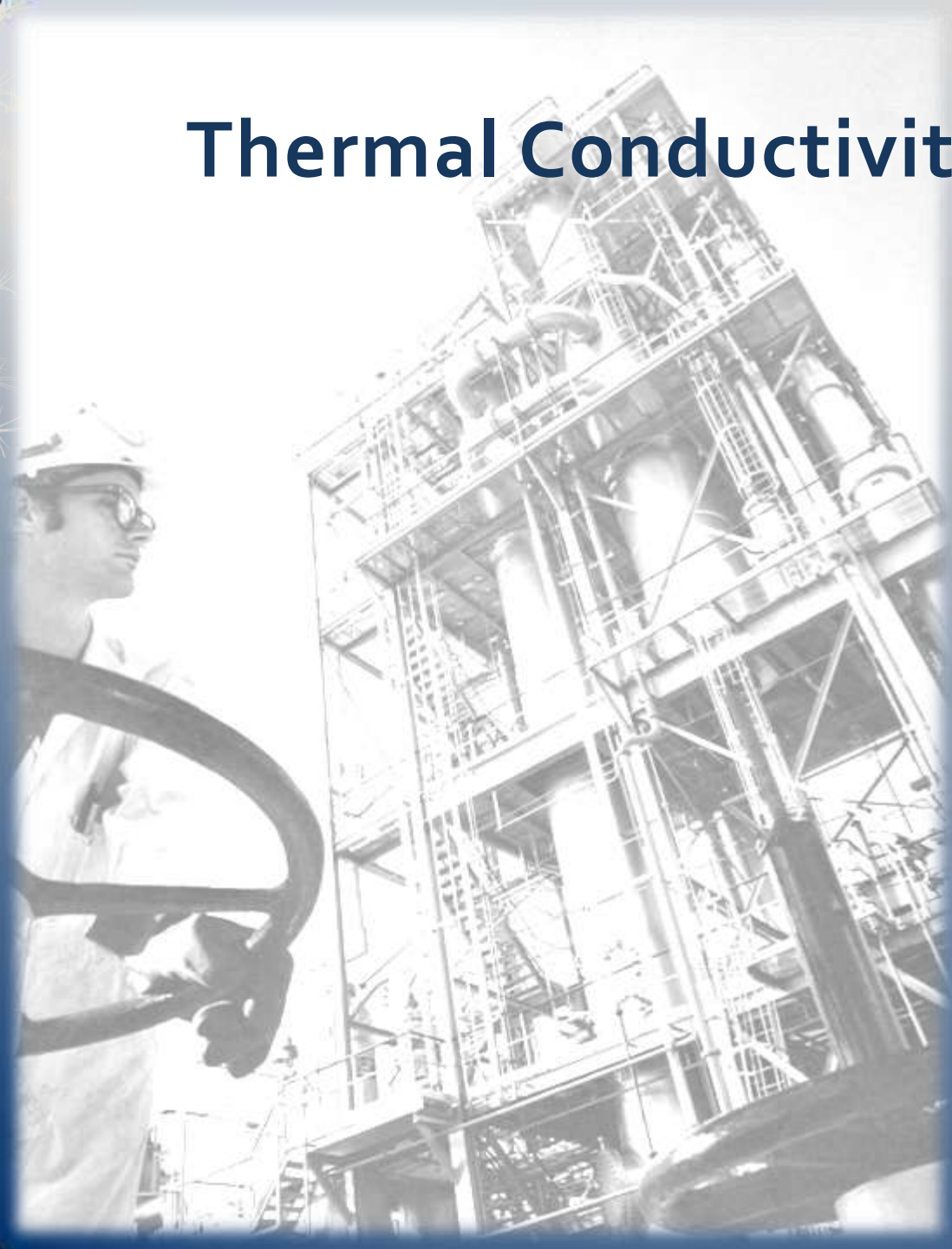
# Experimentation Verses Prediction

# Thermal Conductivity Required for



- Equipment design
- Cost-effective and safe plant design
- Simulation packages
- Scale up
- Calculation of transfer coefficients and dimensionless numbers

# Thermal Conductivity Required for



- Equipment design
- Cost-effective and safe plant design
- Simulation packages
- Scale up
- Calculation of transfer coefficients and dimensionless numbers

# Previous Work Done

- Normal boiling point (Rarey and Cordes 2002 and Nannoolal *et al.* 2004)
- Critical property data (Nannoolal *et al*. 2007)
- Vapour pressures (Nannoolal *et al*. 2008 and Moller *et al*. 2008)
- Liquid viscosity (Nannoolal *et al*. 2009)

# Current Work

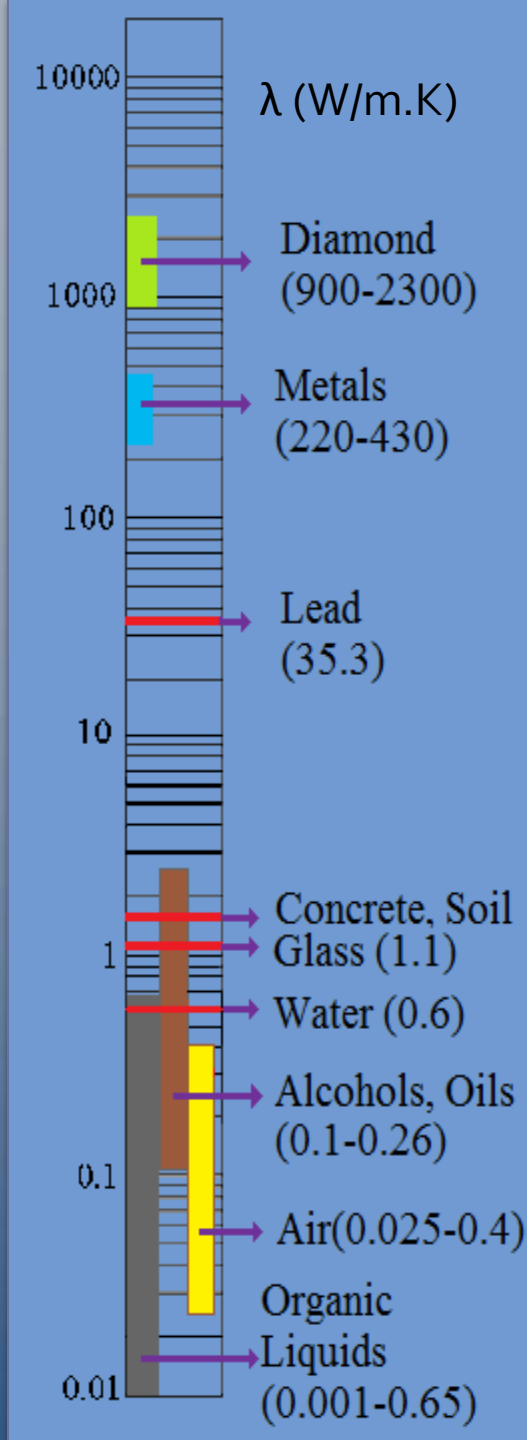
- Bruce Moller – Gamma infinity in water, alkanes, alcohols
- Eugene Olivier – Surface Tension
- Onellan Govender – Thermal Conductivity

# Thermal Conductivity - λ

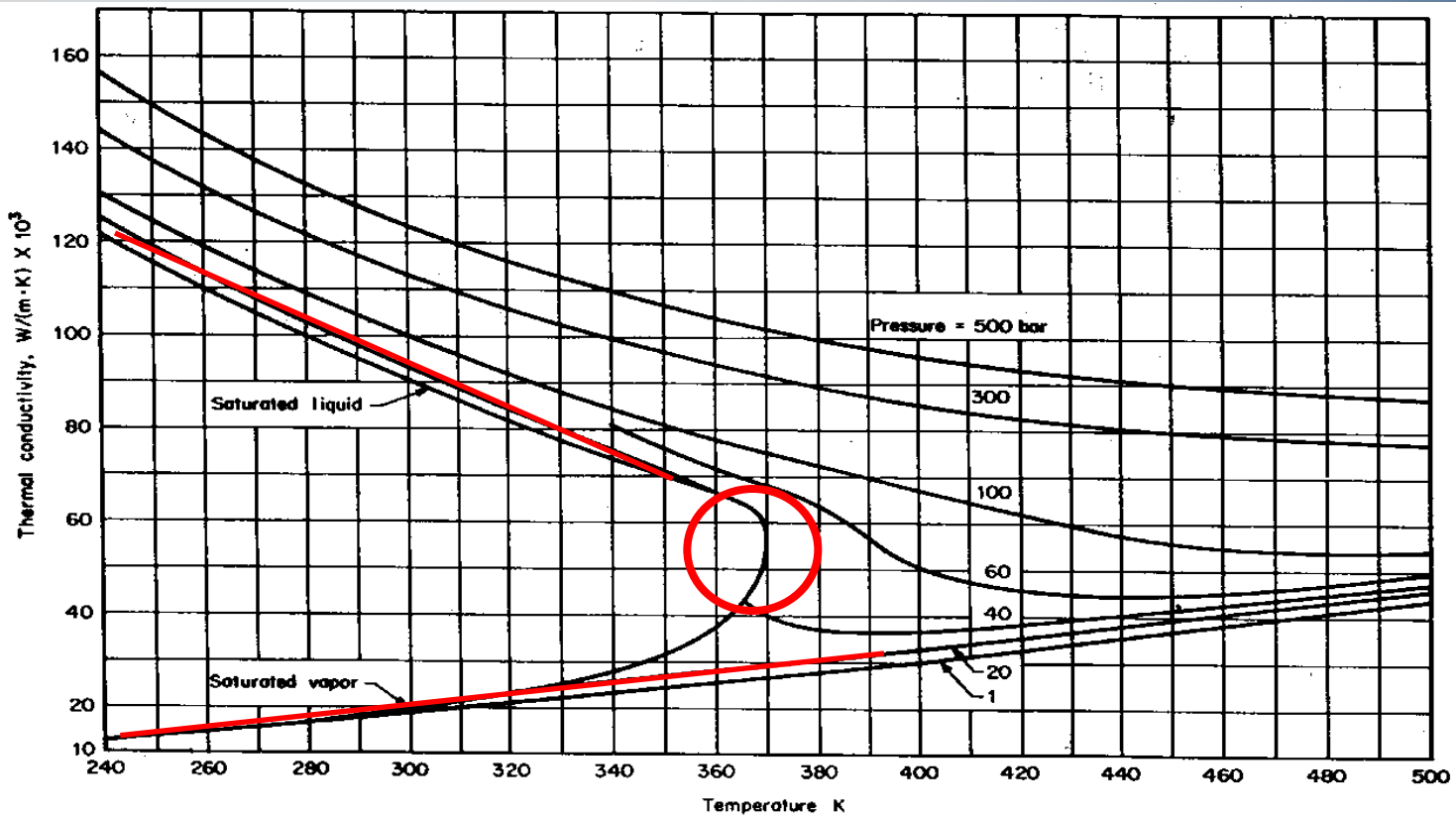
$$J_q = -\lambda \nabla T$$

- Theoretical Contributions and Considerations
- Critical Enhancement

$$\lambda(\rho_n, T) = \lambda_o(T) + \Delta\lambda(\rho_n, T) + \Delta\lambda_c(\rho_n, T)$$



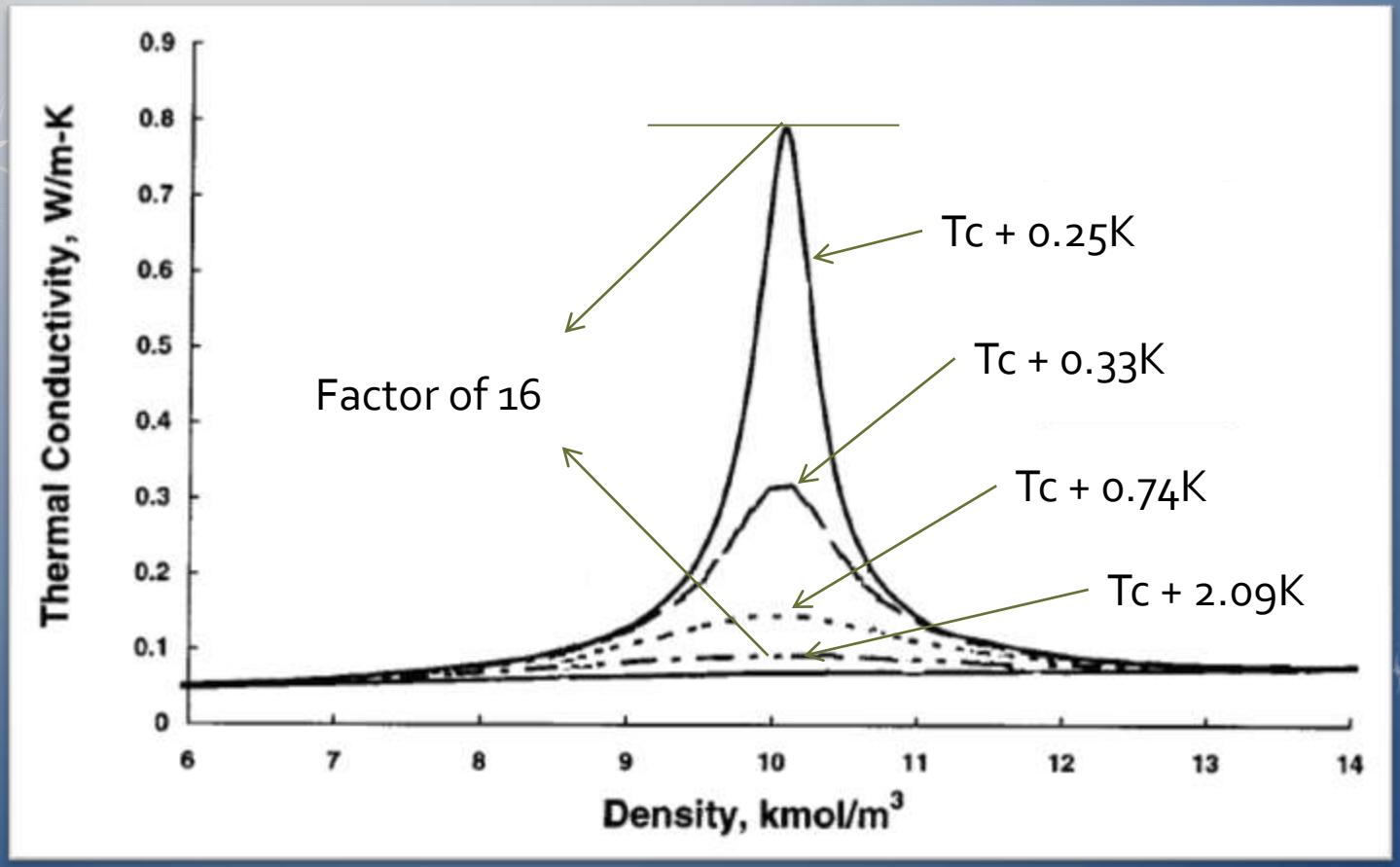
# Thermal Conductivity of Propane as f(T,P)




$$\lambda(\rho_n, T) = \lambda_o(T) + \Delta\lambda(\rho_n, T) + \Delta\lambda_c(\rho_n, T)$$

# Critical Enhancement

Selected isotherms for $CO_2$ depicting the critical enhancement phenomenon (Mathias *et al*. 2002)



# Correlation and Prediction

- Experiments and Data Correlation
- Prediction Models
  - Corresponding States
  - General Correlations
  - Family Methods
  - Group Contribution Method

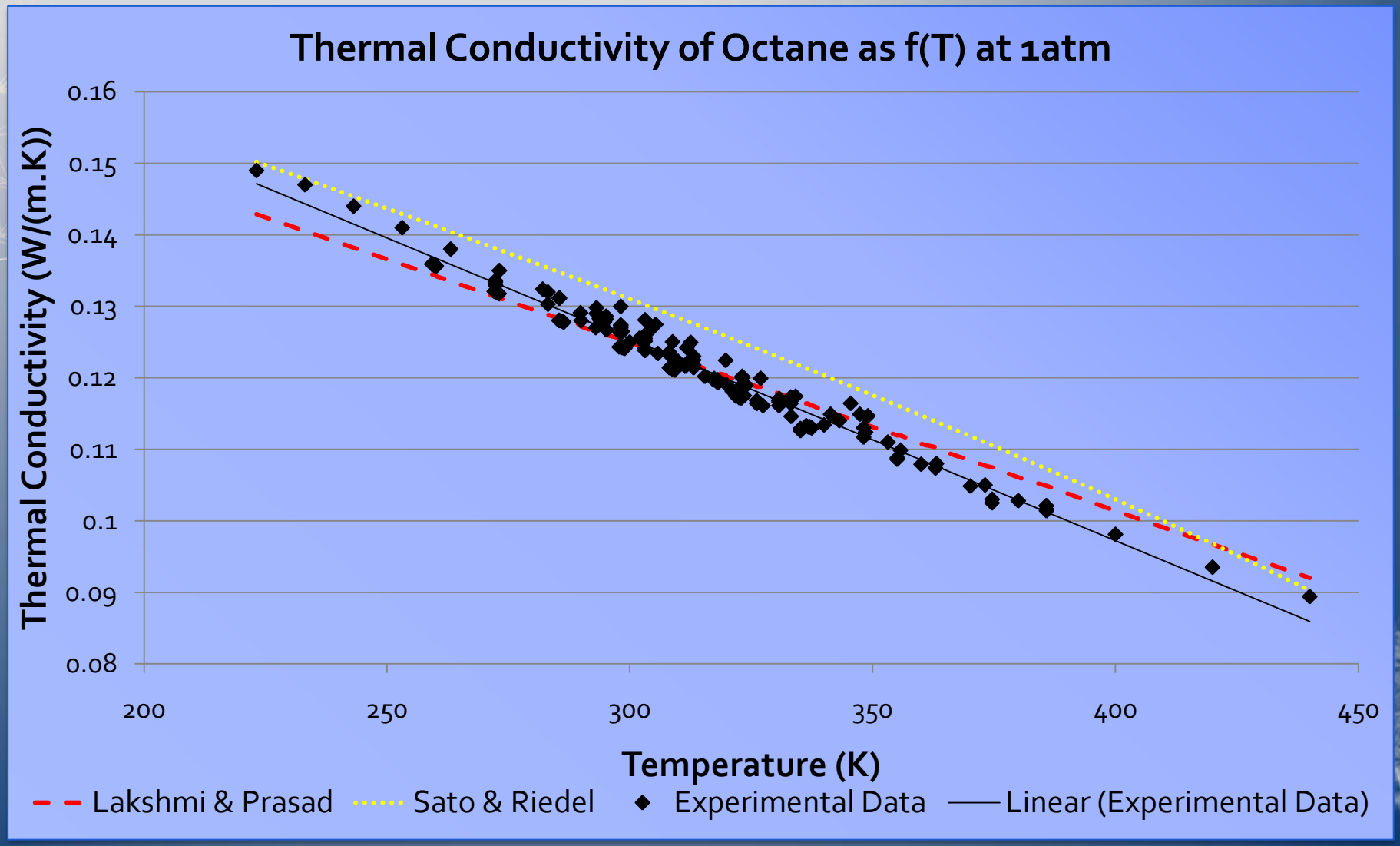
# General Correlation Methods

- Sato and Reidel (1977)
- Lakshmi and Prasad (1992)

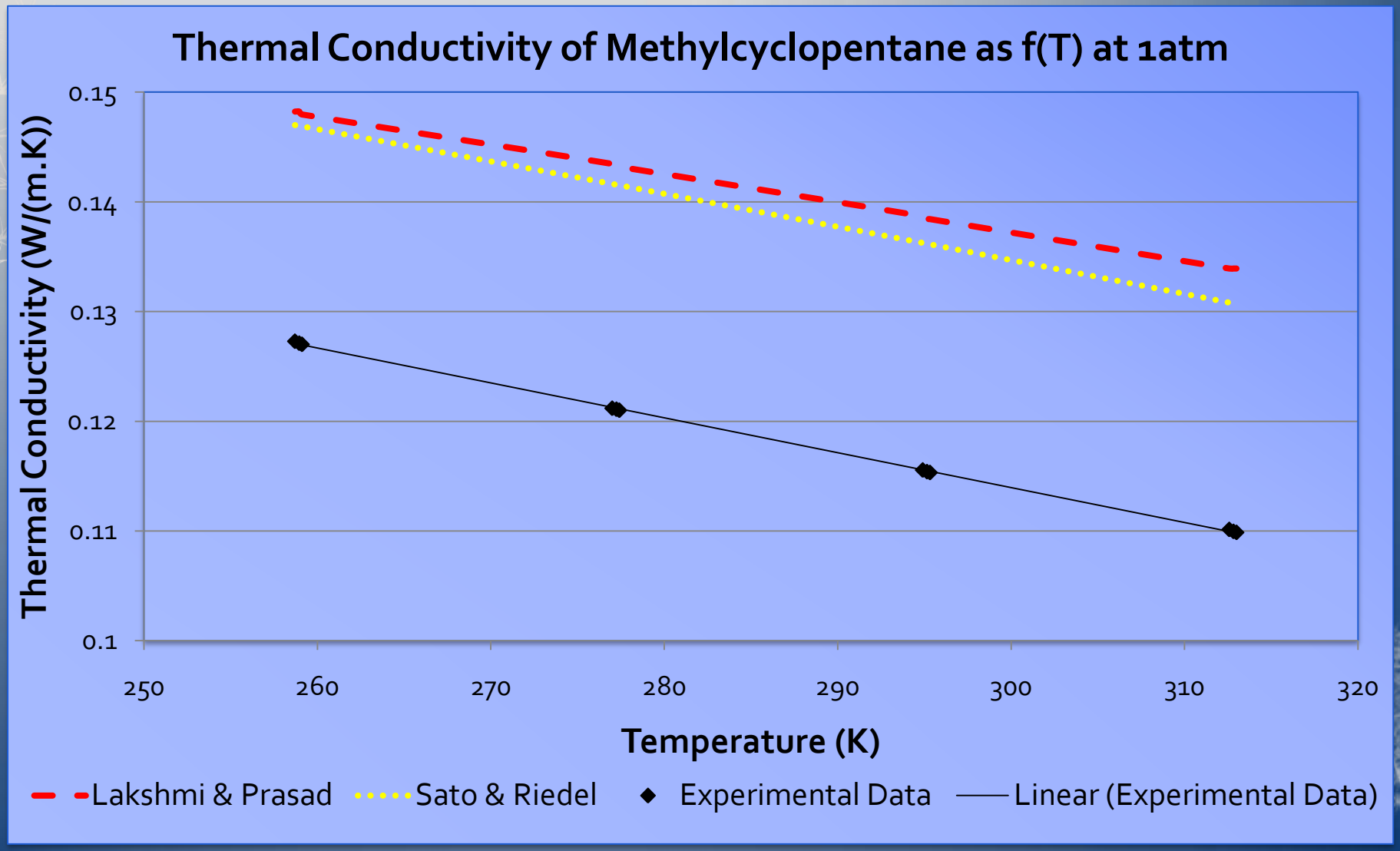
# Family Methods

- Latini *et al*. (1977)

# General Correlation Methods



# General Correlation Methods



# Previous Group Contribution Methods

- Sakiadis and Coates (1955 , 1957)
- Robbins & Kingrea (1962)
- Nagvekar & Daubert (1987)
- Assael, Charitidou & Wakeham (1989)
- Sastri and Rao (1993)
- Rodenbush, Viswanath & Hsieh (1999)
- Sastri and Rao (1999)

# Literature Review & Method Test

| Component Classes | | | |
|---|---|---|---|
| Hydrocarbons | Oxygen Compounds | Ethers | Aldehydes |
| Aromatic Hydrocarbons | Carboxylic Acids | Esters | Nitrogen Compounds |
| Halogen Compounds | Alcohols | Ketones | Amines |

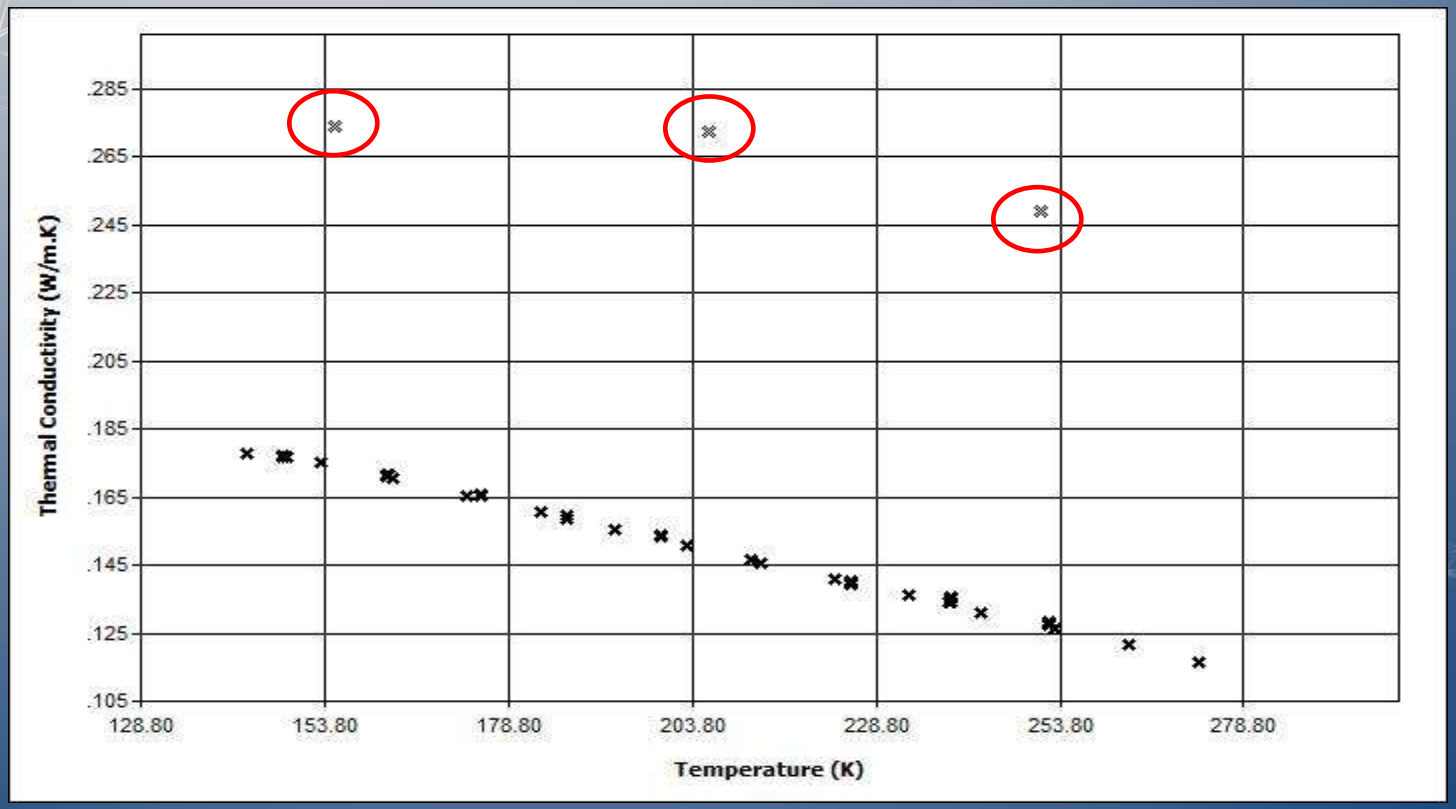
| Methods | Sato & Riedel (1997) | Nagvekar & Daubert (1987) | Lakshmi & Prasad (1992) | Sastri & Rao (1993) |
|---|---|---|---|---|
| RMD (%) | 19.81 | 16.64 | 23.41 | 14.11 |
| Number of Components | 500 | 322 | 500 | 469 |

# Data Filtration and Validation

DDB – 100 515 data points for 876 components

Figure : Data points for n-butane

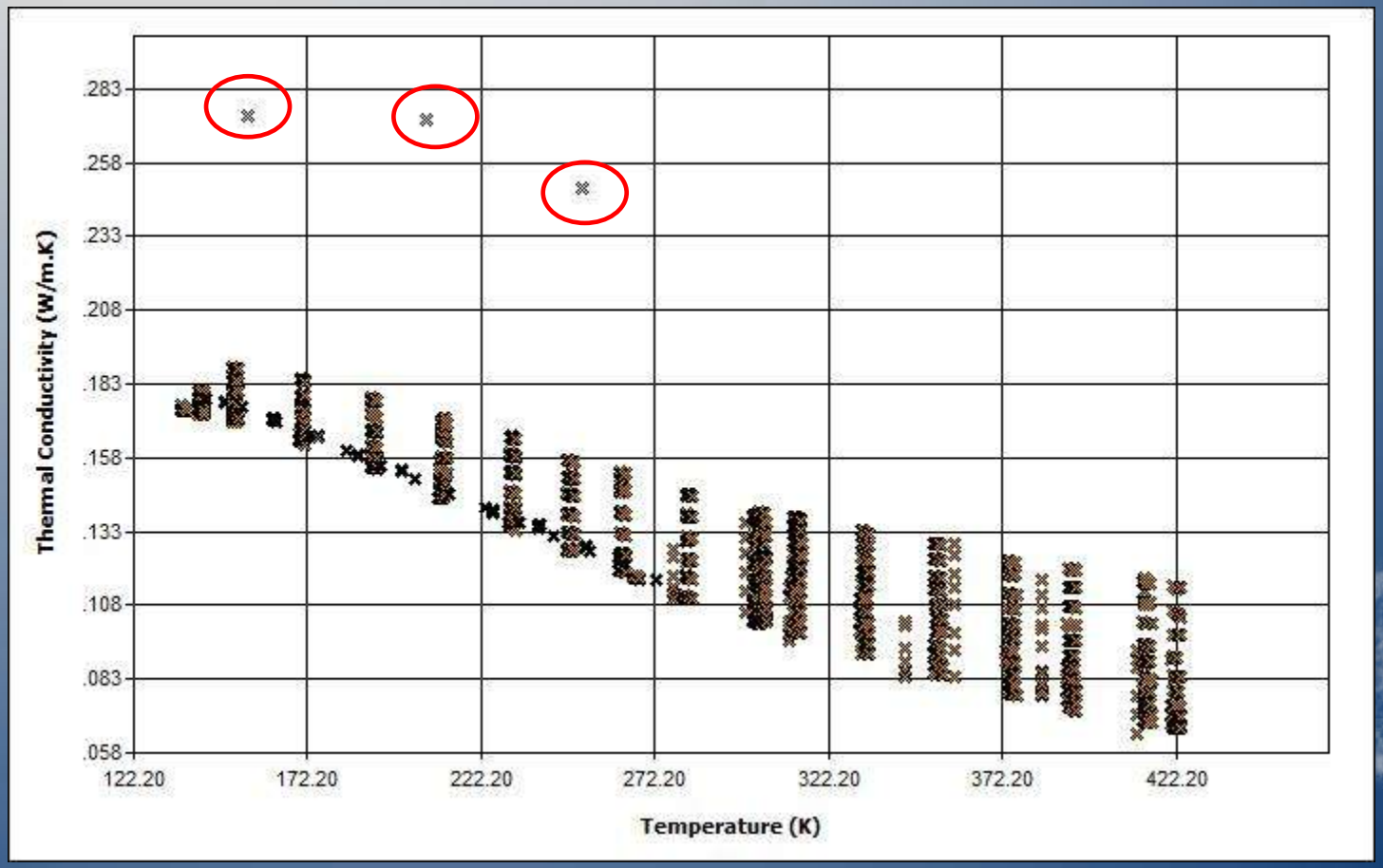
(1atm isobar; 135.75 < T (K) < 272.65)



# Data Filtration and Validation

Figure : All experimental data points for n-butane

(135.75 < T (K) < 423.61; 101.325 < P (kPa) < 70000)



# Model Idea

Separate group contributions for the 3 parts

$$\lambda(T,P) = \lambda(T_{Ref}) \times f(T - T_{Ref}) \times g(P - 101.3kPa)$$

Reference Value

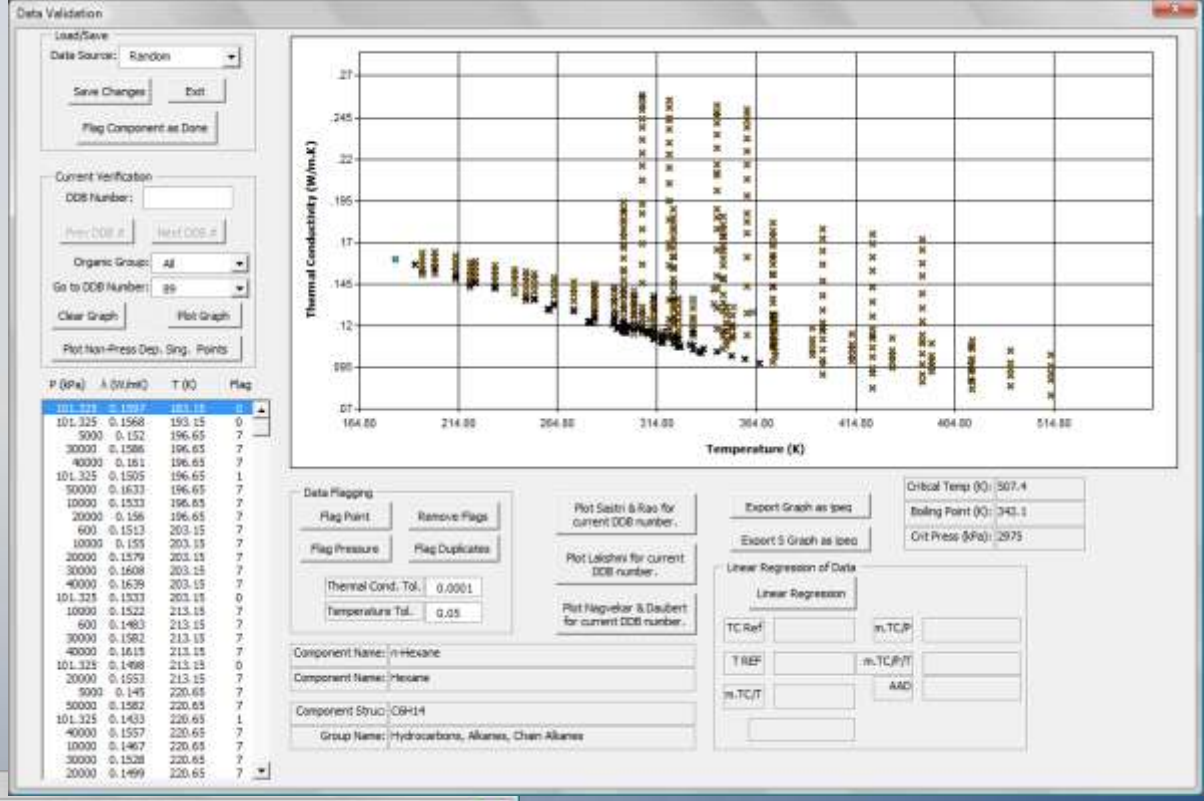
Temperature Dependence

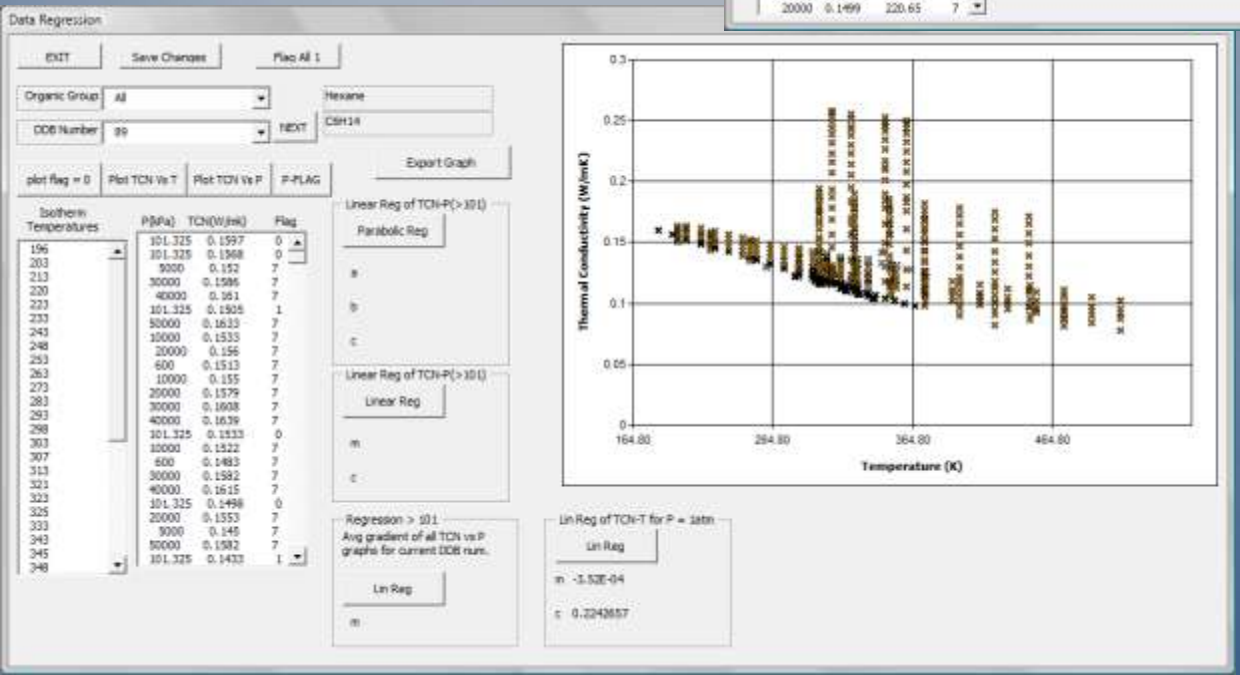
Pressure Dependence

$$\lambda = \lambda_{REF} + (T - T_{REF}) \times \frac{\partial \lambda}{\partial T} + \lambda_P$$

$$\lambda_P = (P - 101.325) \times \left[ \frac{\partial \lambda}{\partial P} + \left( [T - T_{REF}] \times \frac{\partial \lambda / \partial P}{\partial T} \right) \right]$$

# Software Development




- The DDB (Artist)
- Microsoft Office
- SQL & ADO

# Future Work

- Select a regression model and determine empirical parameters for all compounds
- Evaluation & definition of structural groups
- Regression for structural or bond contributions
- Testing using a test set of thermal conductivity data
- Optimisation of structural or bond contributions

# Summary

- Importance of prediction methods
- Thermal Conductivity
- Review of available prediction methods
- Evaluation of methods
- Filtration and validation of data from DDB
- Software
- Work left to be done

# Acknowledgements


- Prof. D. Ramjugernath from UKZN
- Prof. J. Rarey and Prof. J. Gmehling from Oldenburg University
- Bruce Moller and Eugene Olivier
- DDBST Software and Separation Technology
- South African NRF and German DLR (BMBF)