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Pifalls when doing thermodynamic modeling in E&P application.

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Journées Thermodynamique des Sous-Sols (SFGP)

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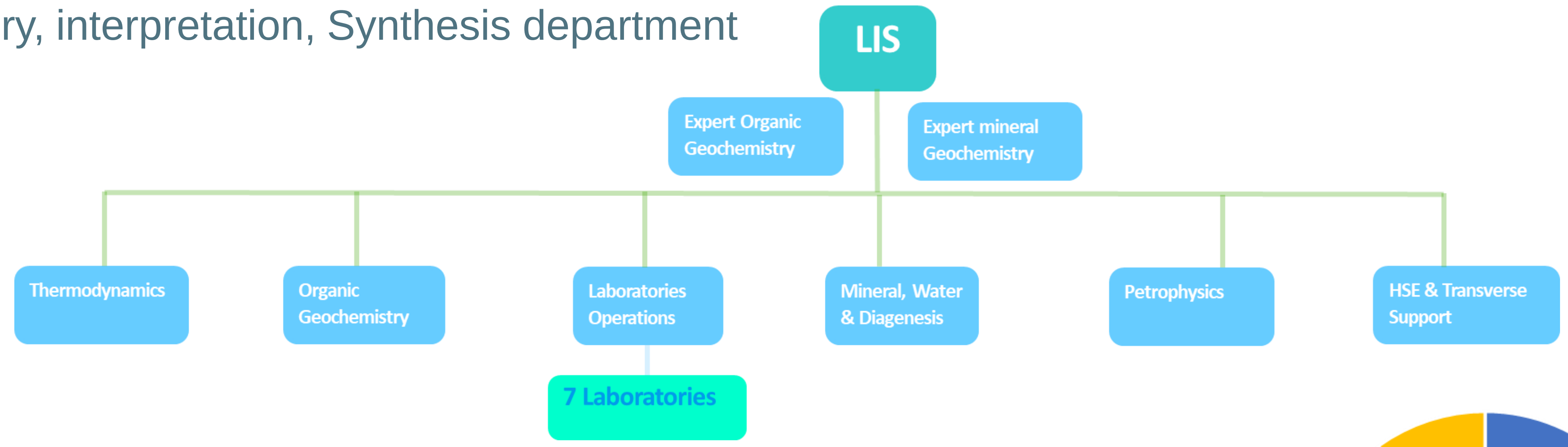
01.

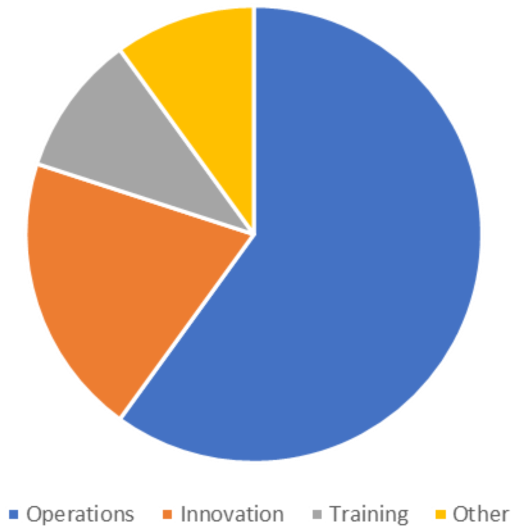
Thermodynamic modeling for E&P

PVT and thermodynamic department at TotalEnergies

- Laboratory, interpretation, Synthesis department



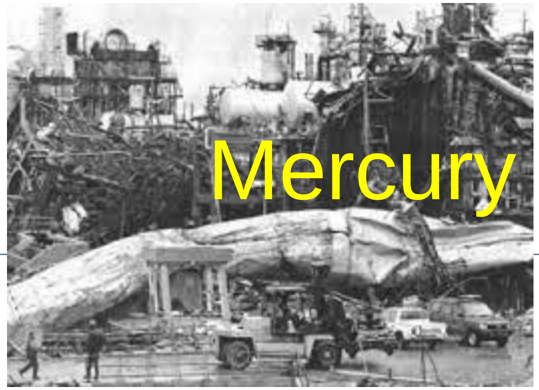
- **At the heart of the measure (fluid, rock, material) and its interpretation → Strong business impact**
- **Evaluate Discoveries and Optimize Field development & CCS**
- **Maximize Field performances**
- **Surface facilities design and Well integrity diagnosis for remedial**



Properties of interest

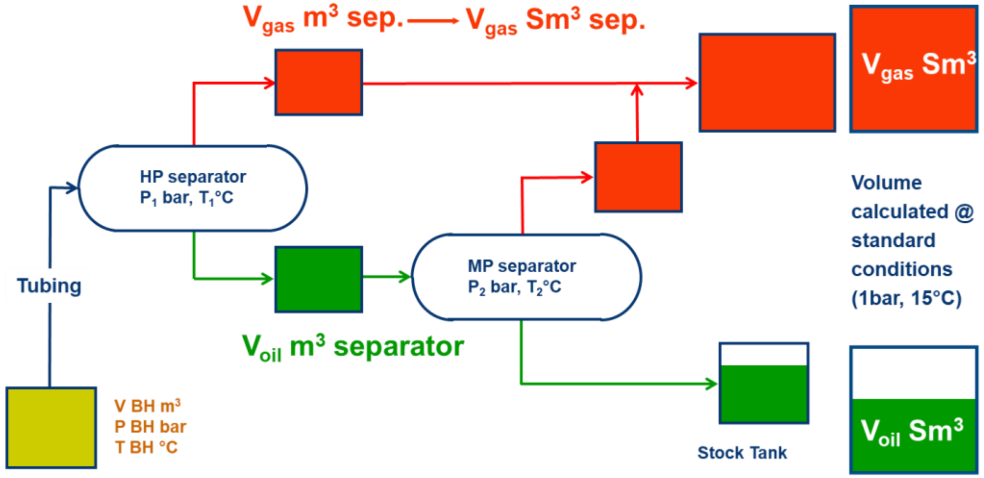
- Thermophysical properties
  - Isothermal compressibilities
  - Viscosity
  - Density
- Phase enveloppe, saturation pressure
- Composition
  - HC composition, paraffins, asphaltenes
  - Inert gas: N2, He
  - Acid gases : H2S, CO2
  - Trace elements

Downgraded HC value (economics), causes production issues



Properties of interest

- Basic production data (surface)



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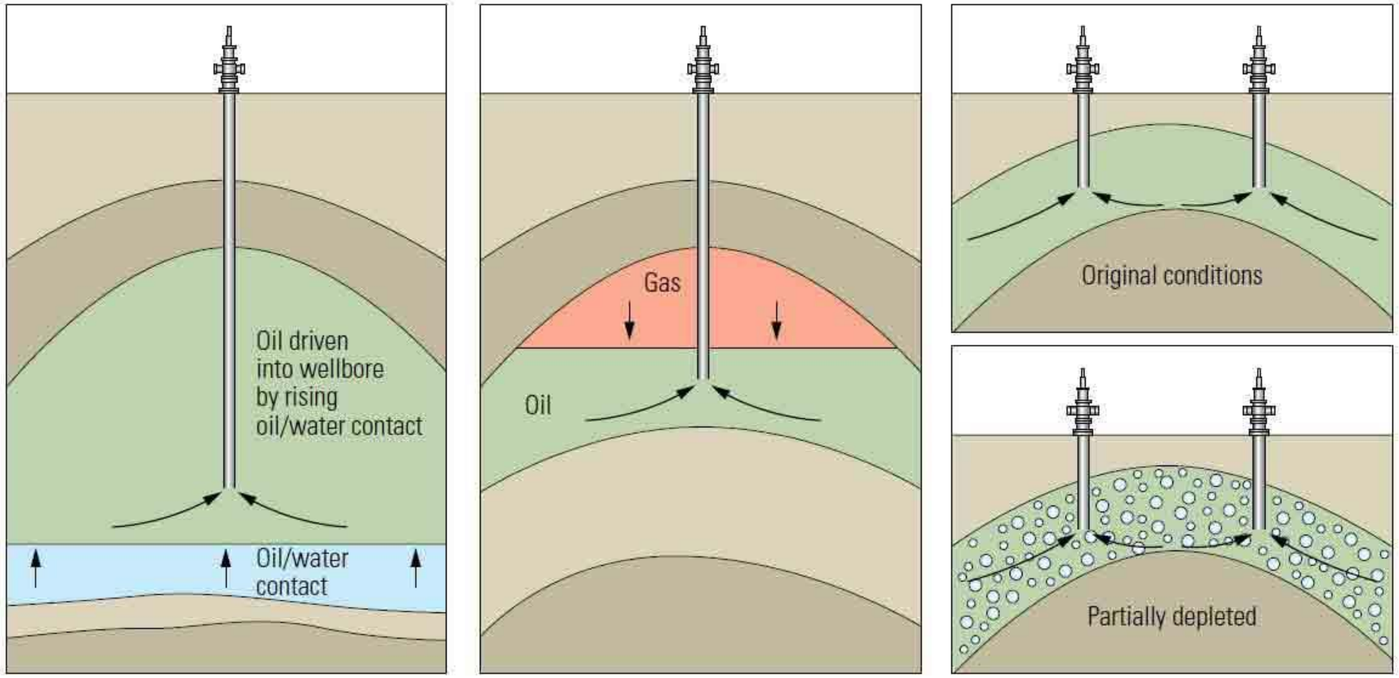
Properties of interest

- Reservoir monitoring data (downhole)



Modeling, but for which purpose / client ?

- Thermo Modeling using cubic EOS (PR-78 mostly)
  - **Happy with that!**
  - Strong know-how on model calibration
  - Used in reservoir modeling softwares

The experimental and mondeling study mostly consist in providing **SIMPLIFIED** fluid model for fluid mechanics simulations!

Black-oil simulations (60% of reservoirs)

- Tabulated value for Psat, GOR, Bo, viscosity vs P

Compositional model ie cubic EOS (40% of réservoirs)

- EOS with 8-12 pseudo components

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With which tools / models ?

- Cubic EOS (PR, SRK) mostly (Soreide-Whitons occasionnaly)
  - Full models (50+ cpds) for internal use and lumped model (8-12 pseudo-cpds) for reservoir modeling
  - Diphasic flash (mostly), even if polyphasique available (internally)

- Dedicated thermodynamic modeling software adapted to petroleum industry
  - BEST (internal development)
  - PVTSim
  - PVTp, Eclipse,…

- Main pitfalls for our activities so far:
  - Analytical characterization
  - Uncertainties management
  - Heavy cpds thermodynamic properties
  - Thermodphysical properties modeling

➔ To be honest, we are a bit late on New energy stuffs that require more complex modeling models

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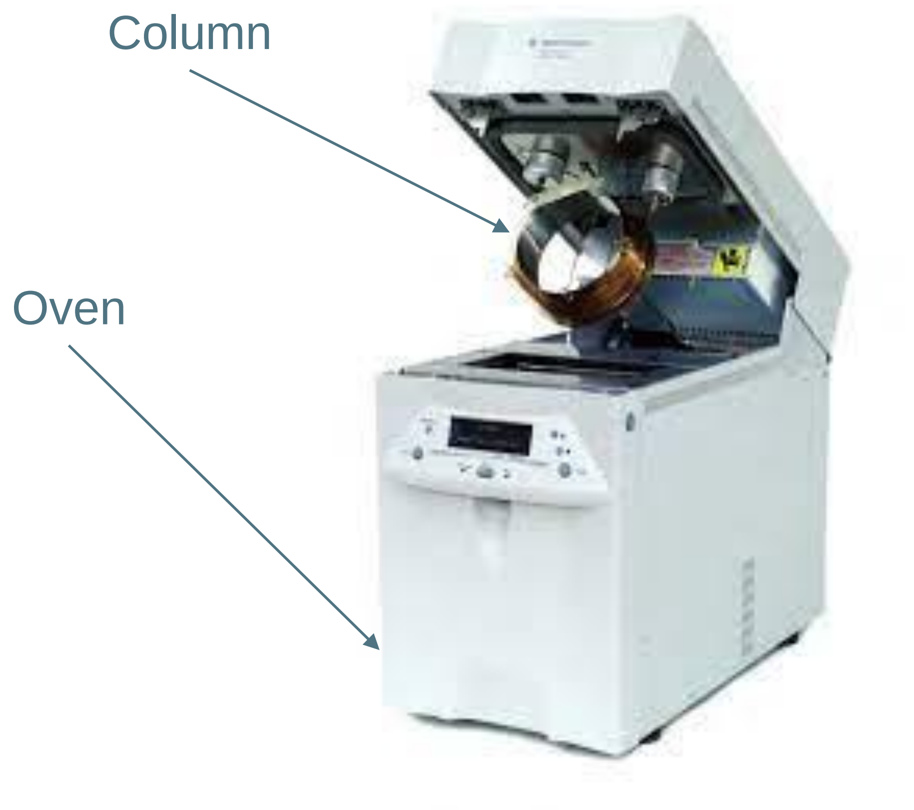
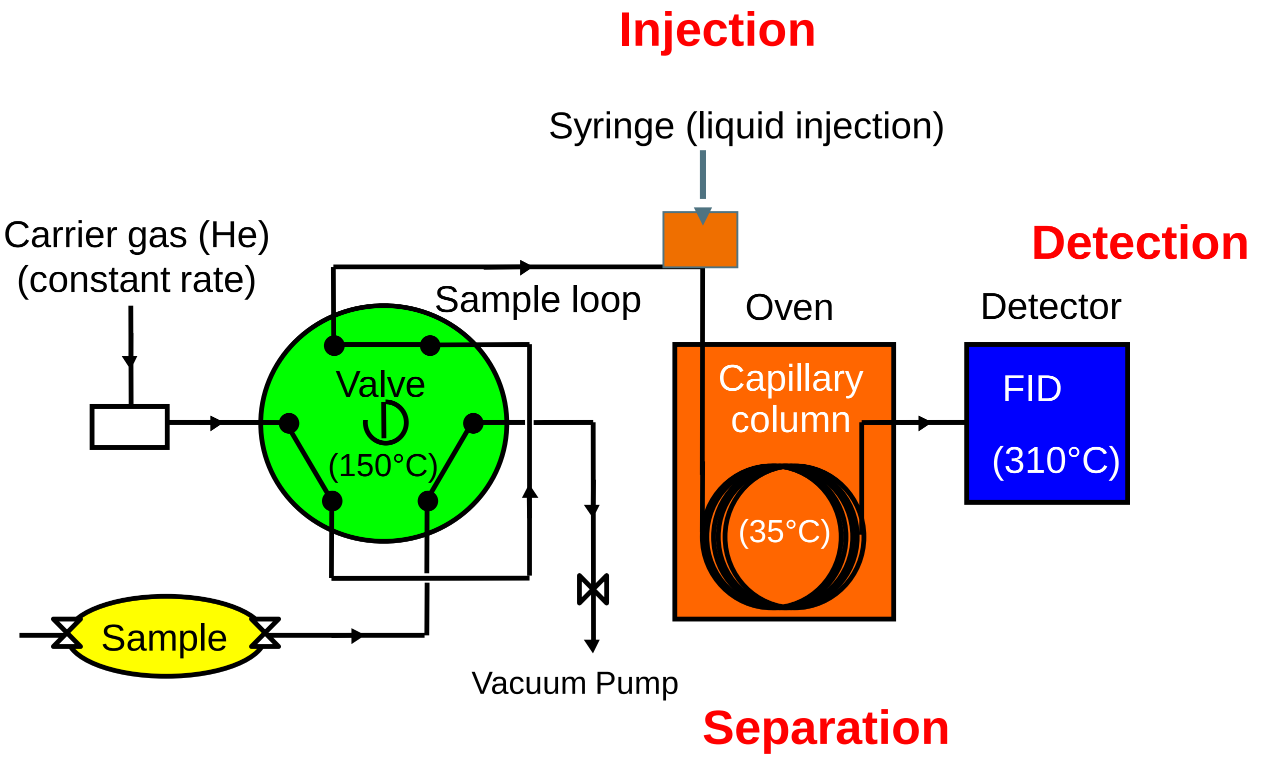
02.

Analytical charaterization

For thermodynamic modeling applications

Apparatus (e.g. agilent 6850)





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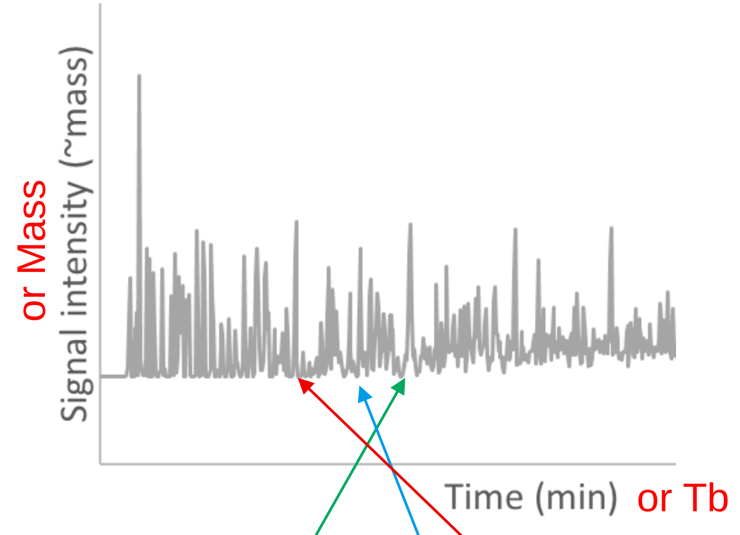
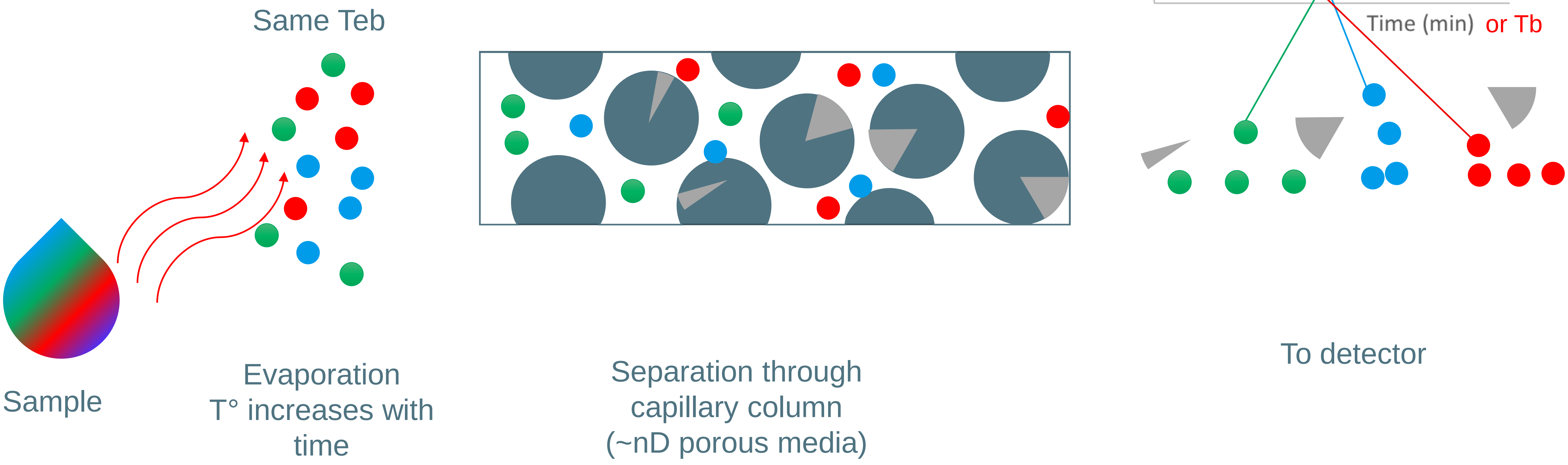
Principle of Chromatographic Analysis (GC)

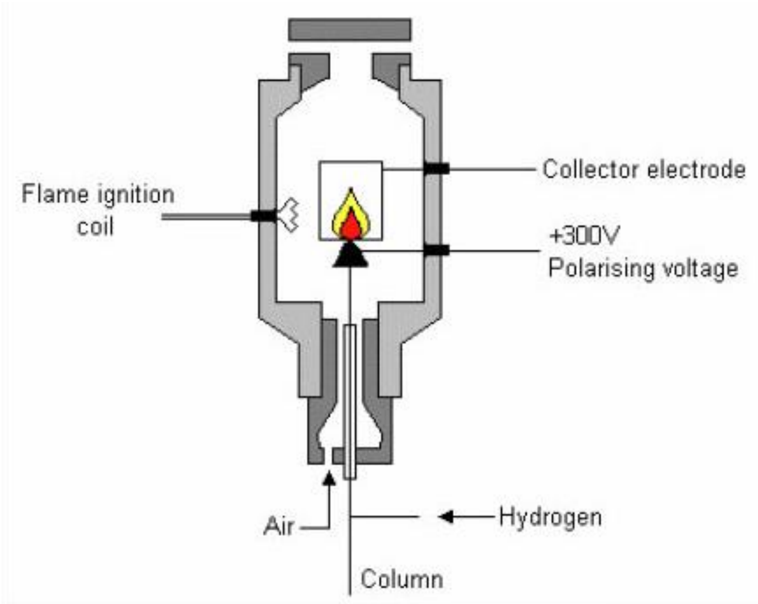




Two types of detectors used

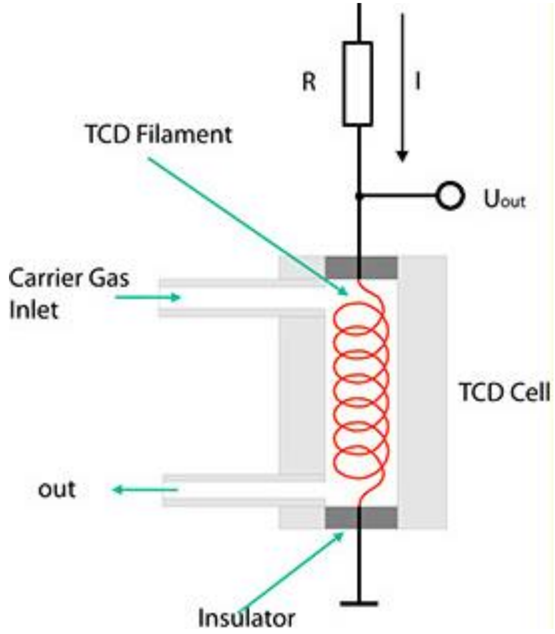
FID : Flame ionisation detector

- Measure C* released by « burning » the effluent molecules
- For HC (ie molecules that « burn »)



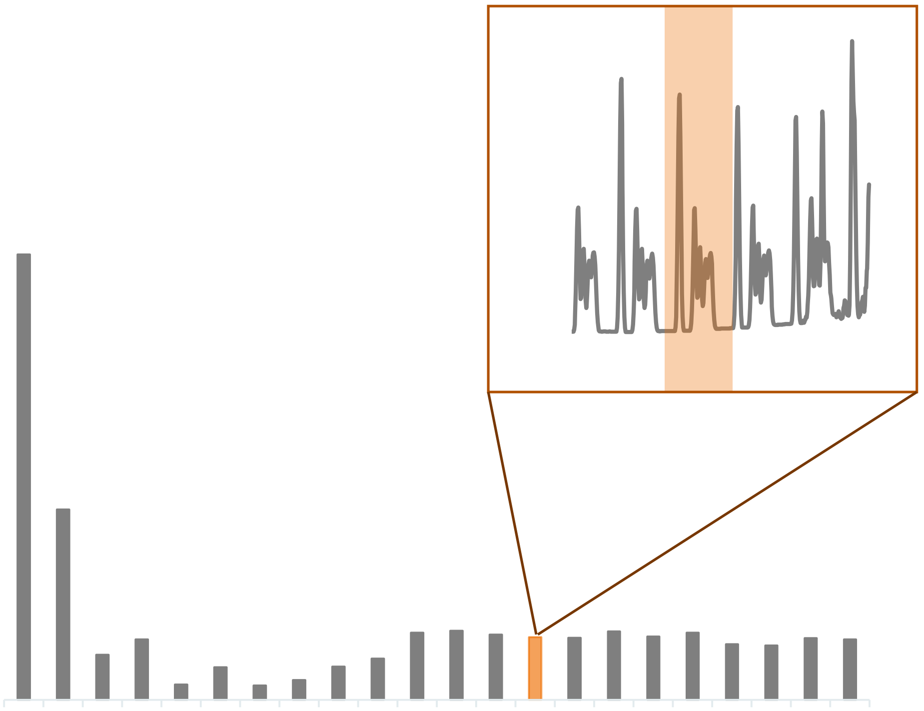
TCD : Thermal conductivity detector

- Change of filament T° due to molecules types and concentration
- For inert gases (ie N_2, CO_2) and light HC (C_1-C_3)

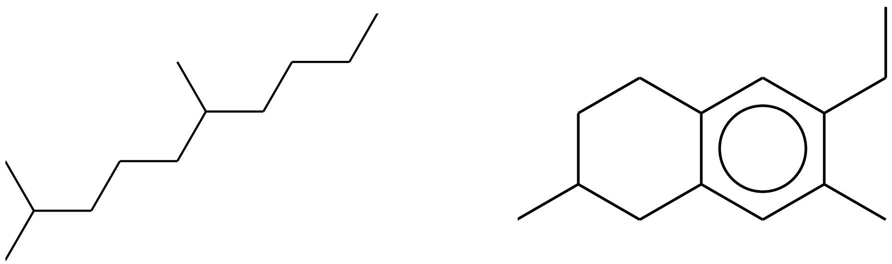


⚠ Detector calibration needed

Oil composition : textbooks vs reality

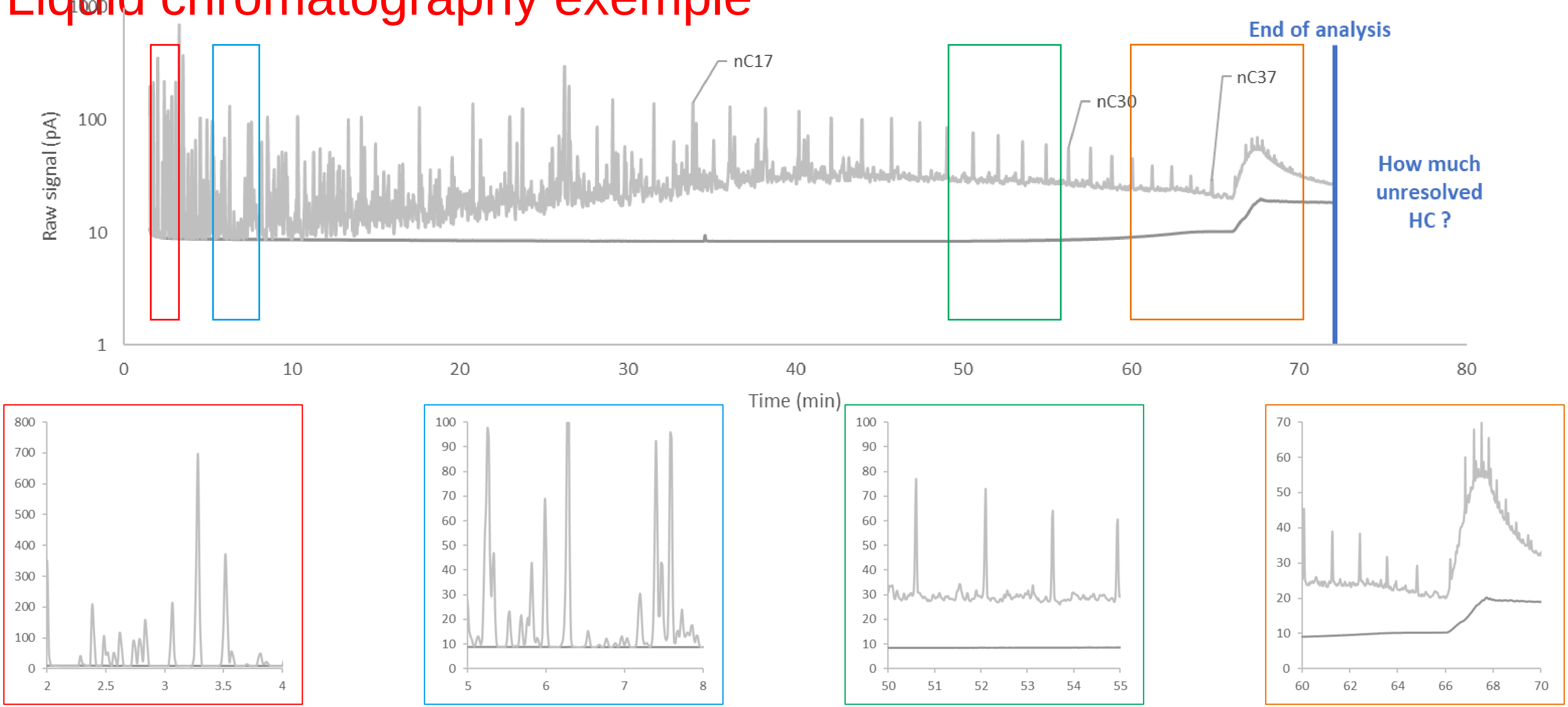

Petroleum fluid composition

- Components in heavy cuts ?



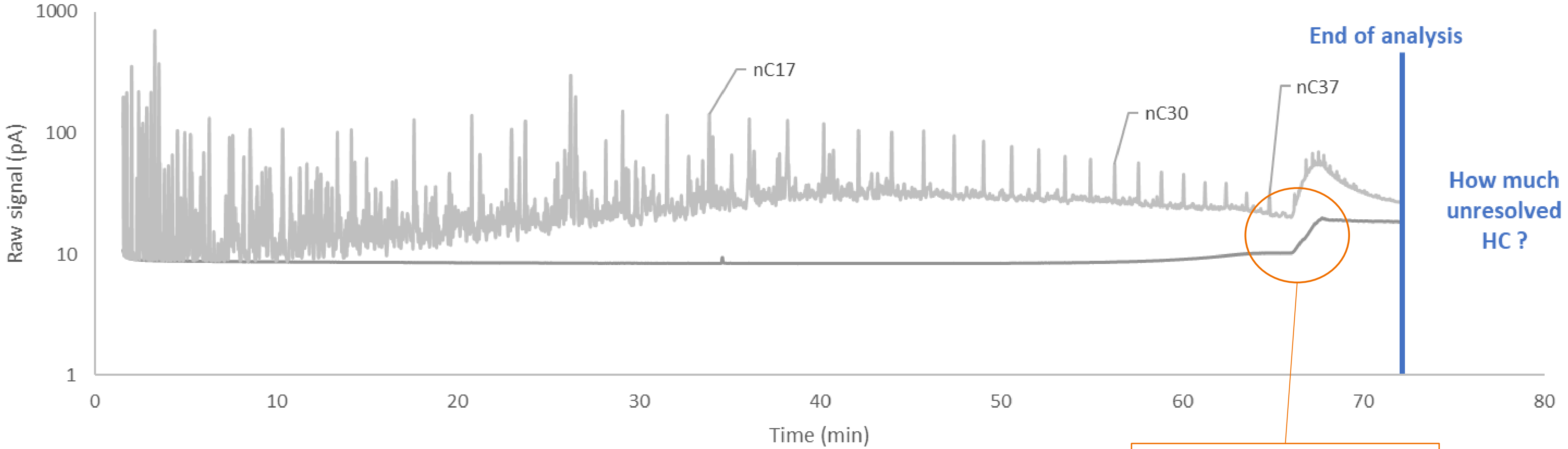
- Hundreds to thousands of **unresolved** components in oil
- Pure components (PC) correspond to a single peak
- Pseudo-component Cn is a PC « cluster » defined has : Tb (C_{n-1}) < Tb (HC) ≤ Tb (C_n

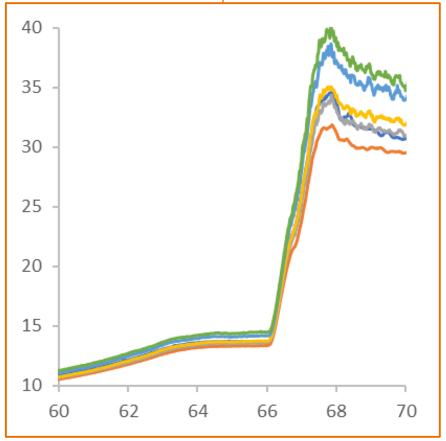
Liquid chromatography exemple



- *Unresolved HC varies from ~ 0 to 50%mass*

Liquid chromatography exemple





- Unresolved HC fraction varies from ~0 to 50%wt
- Impact of baseline shifts
- Response coefficients
- Internal standar

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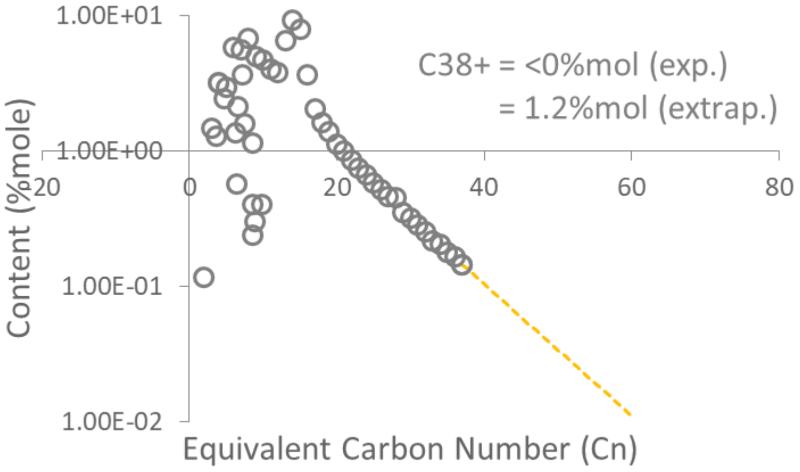
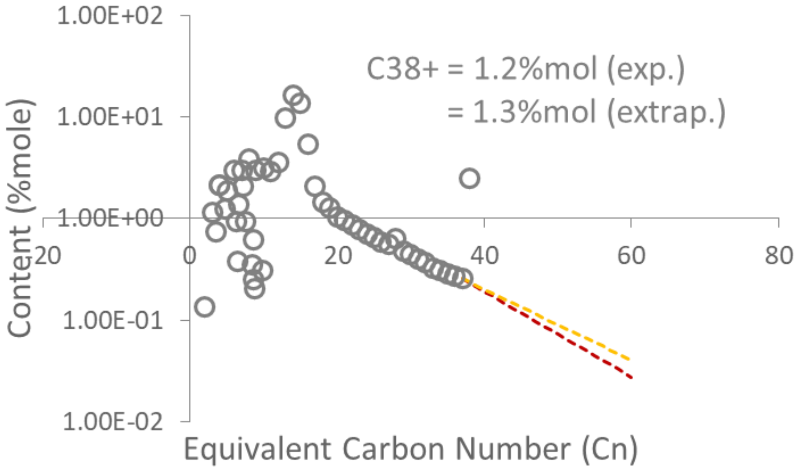
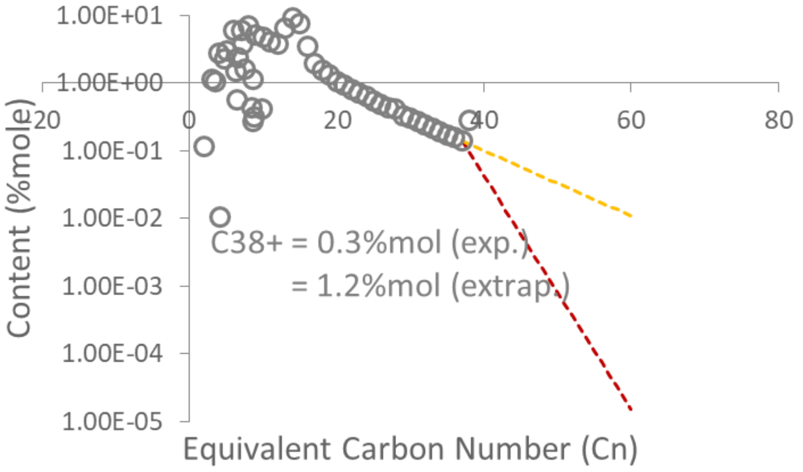
Impact of oil composition in practice



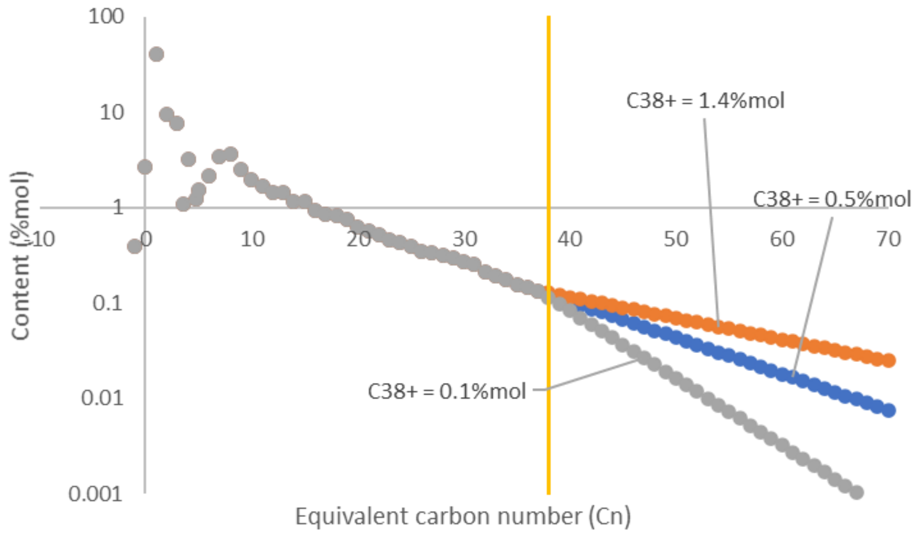


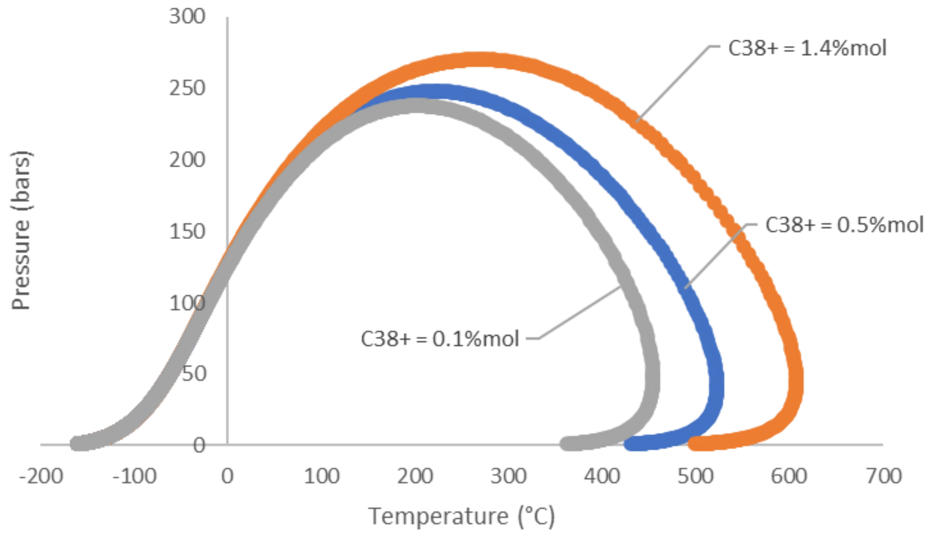


- Repeated experiments on 3 different fluid samples coming from the same reservoir, same depth. They should be identical

Impact on phase equilibria

- Classical oil, GOR = 200, Psat = 233bars @ Tres / Pres





Huge impact of very small amounts of components. Whats for impurities in CCUS context?

How confident are we on paramters with CCUS Eos such as GERG-2008?

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03.

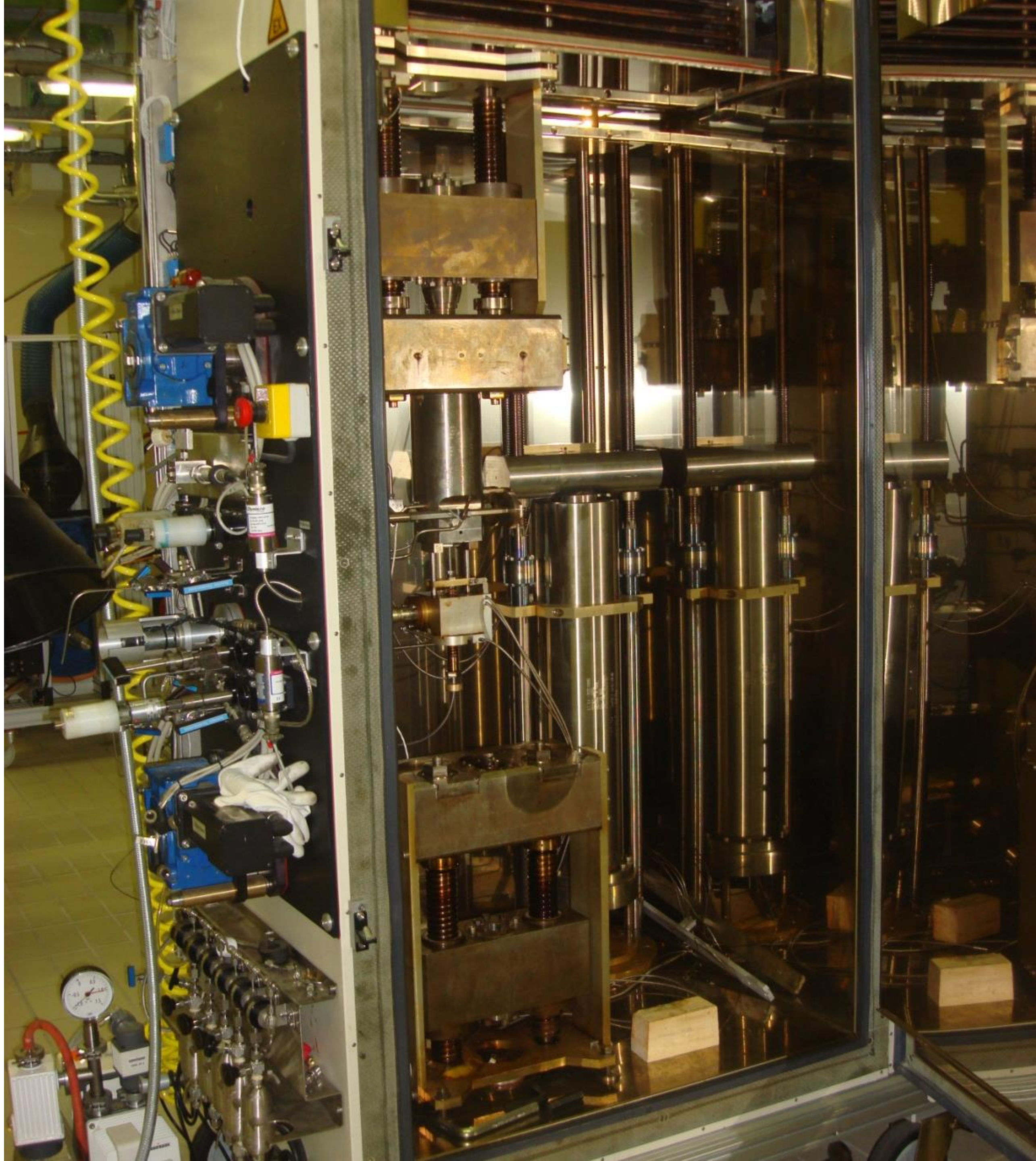
PVT data experiments

When total uncertainties are bigger than the advertised ones.

PVT unit performances

- **Range of work**
  - Pressure : 1 bar - 2000 bar
  - Temperature : -20°C to 200°C
  - GOR : 5 to 2000 m3/m3
  - Viscosity : 0.2 to 200 cPo

- **Accuracy**
  - ⇨ Volumes ± 10^{-3} cm3
  - ⇨ Temperature : ± 0.2°C
  - ⇨ Pressure :
    - HP : ±1 bar
    - BP : $\pm 10^{-3}$ bar
  - ⇨ Viscosity : $\pm 10^{-2}$ cPo



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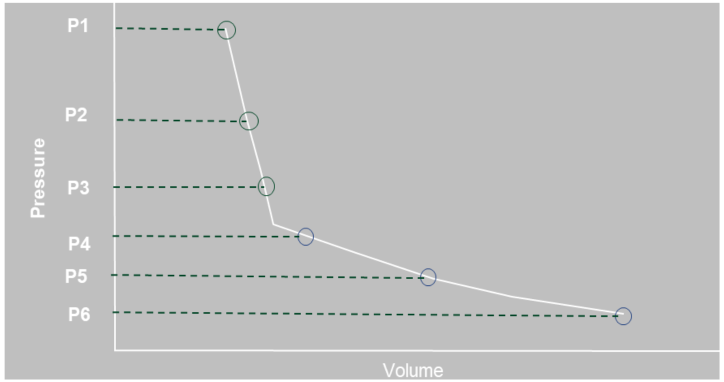
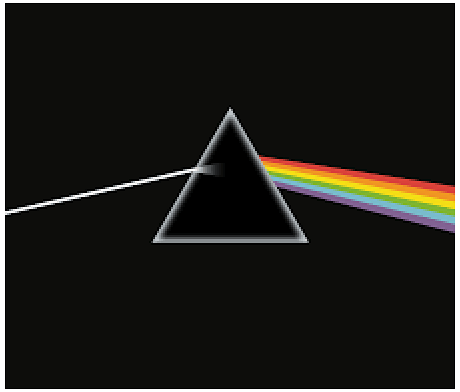
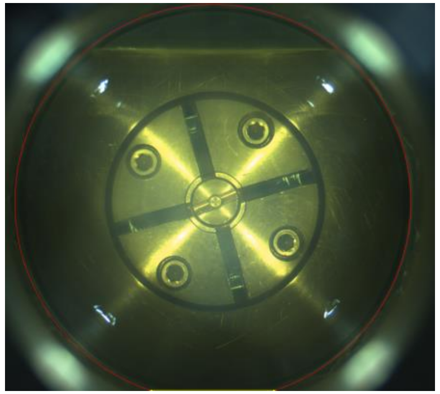
Phase enveloppe

- Phase enveloppes are not measured in the lab!
  - ➔ Few Psat @ various temperature + fitting
- Different methods can be used:
  - P/V curve fitting
  - Optical detection
  - Droplet appearance

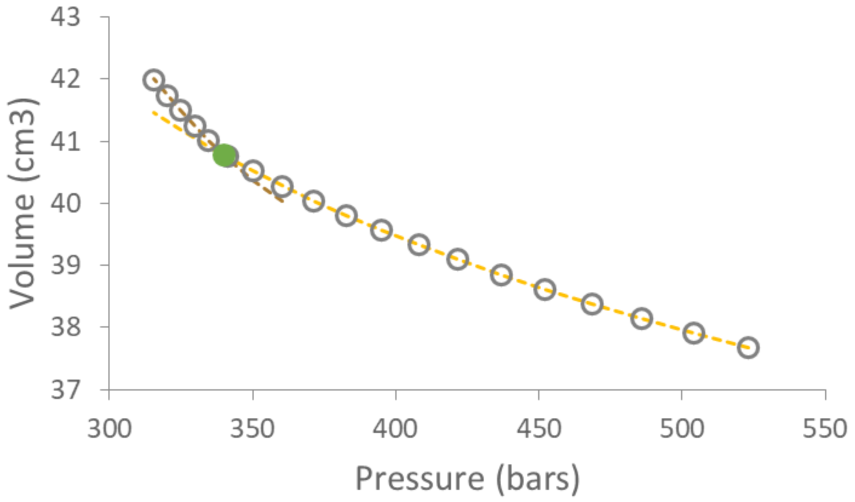


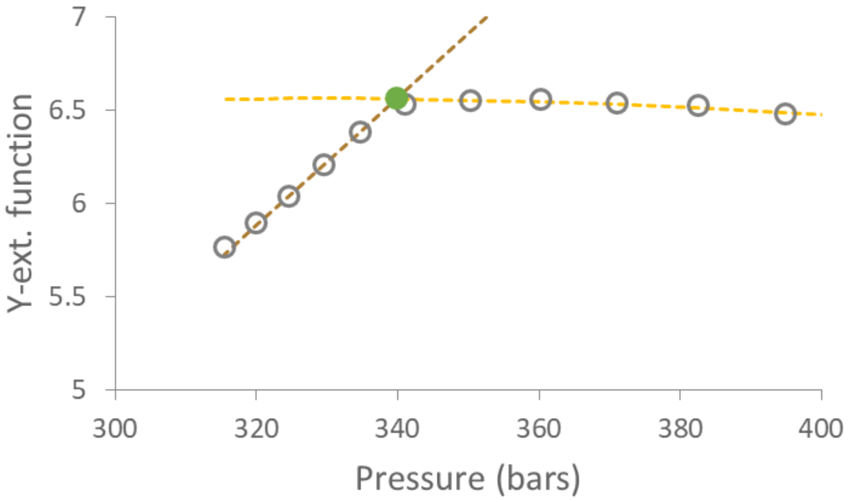




Phase enveloppe

- Uncertainties estimation on P/V curve (GOR = 410 Sm3/Sm3, ρ_{res} = 540kg/m3):
  - Intercept of liquid and diphasic behavior on Y-ext plot





- Experimental uncertainties: P ~ 1bar, V ~ 1µl
- Uncertainties on Psat using MC algorithm

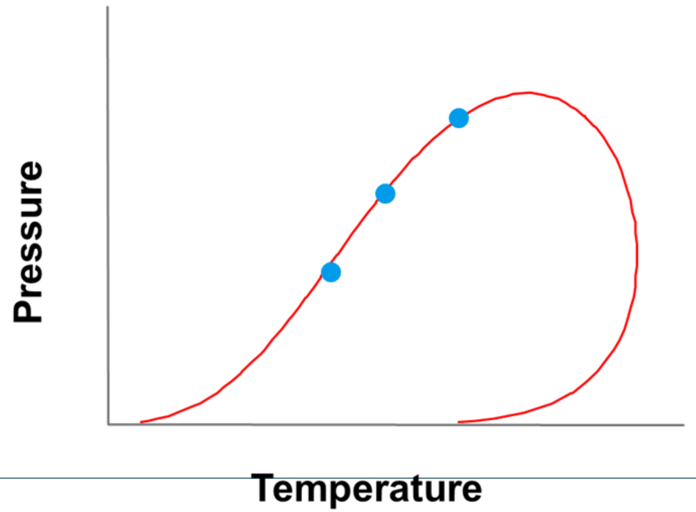
	Psat (bars)	ChiT (bars-1)
moyenne	339.5	0.00049
Etype	3.8	5.6E-06
Etype (%)	1.1	0.08

Phase enveloppe

But:

Temp. (°C)	Psat (bars) P/V curve	Opt. Mtd	Drop.
109	335.8	337.5	
115	339.1	337.9	340.8
145	334.5	337.2	342.9

- Which one to trust ?
- What could be the impact on the calculated phase enveloppe ?



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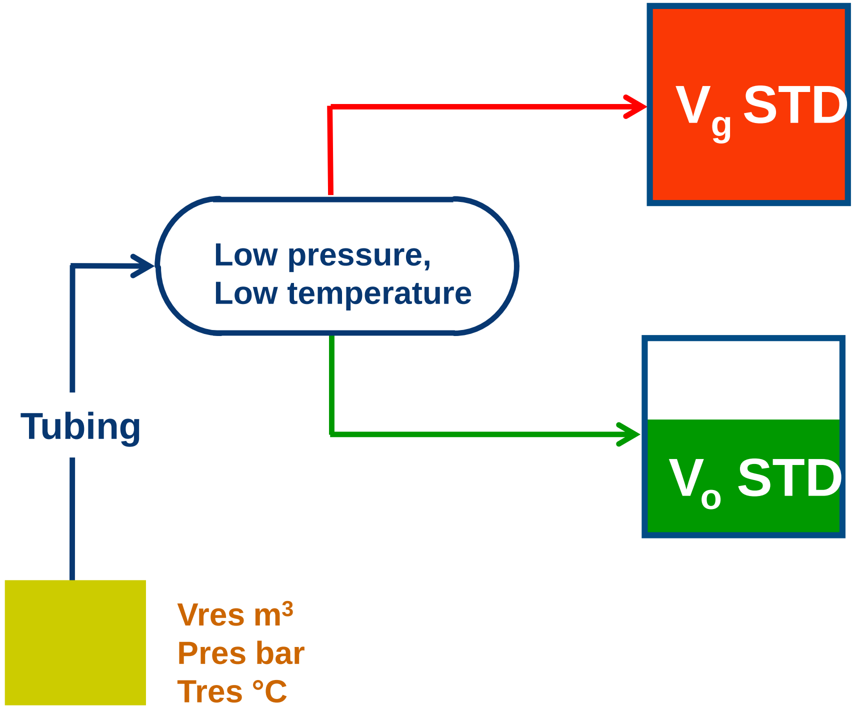
Flash test experiment (for an oil)



Volumetric properties:

$$GOR(Sm^3/Sm^3) = \frac{V_{g,STD}}{V_{o,STD}}$$

$$B_o(Rm^3/Sm^3) = \frac{V_{res}}{V_{o,STD}} \geq 1$$

Phase densities:

$$API = \frac{141.5}{\rho_{o,STD}} - 131.5$$

$$S_g = \frac{\rho_{g,STD}}{\rho_{air,STD}}$$

Mass balance:

$$\rho_{res} = \frac{\rho_{o,STD} + GOR \times \rho_{g,STD}}{B_o}$$

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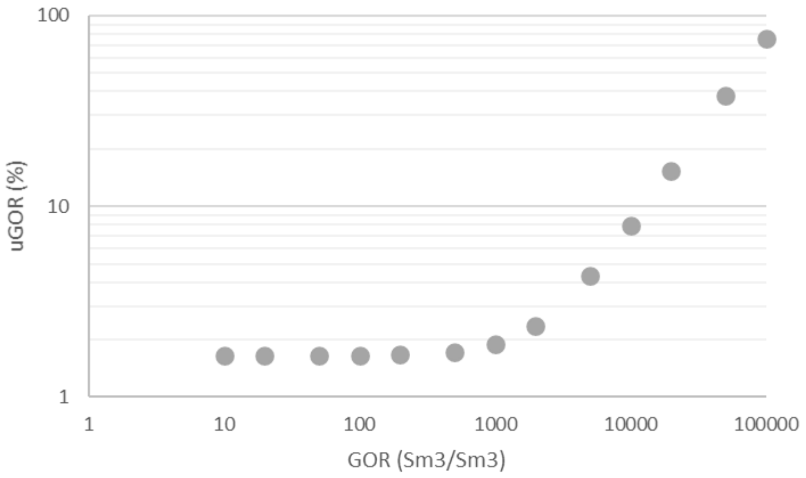
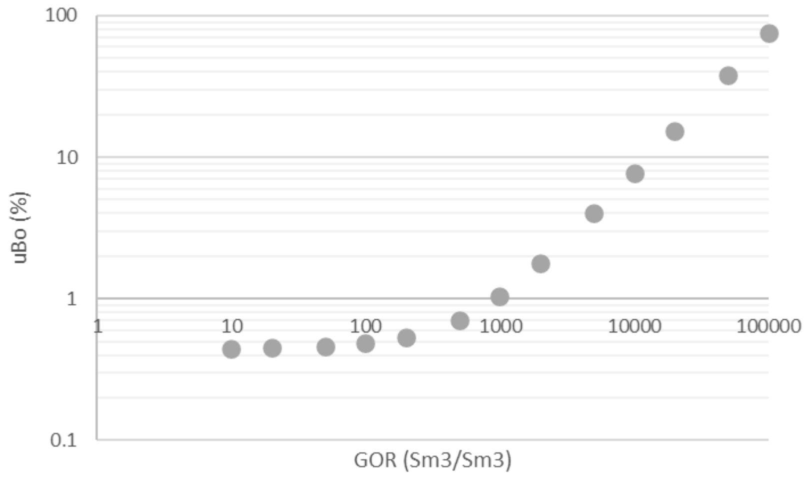
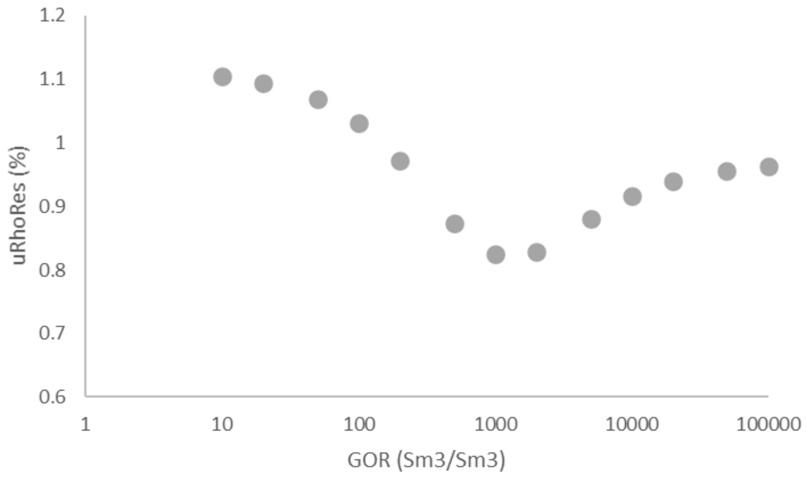
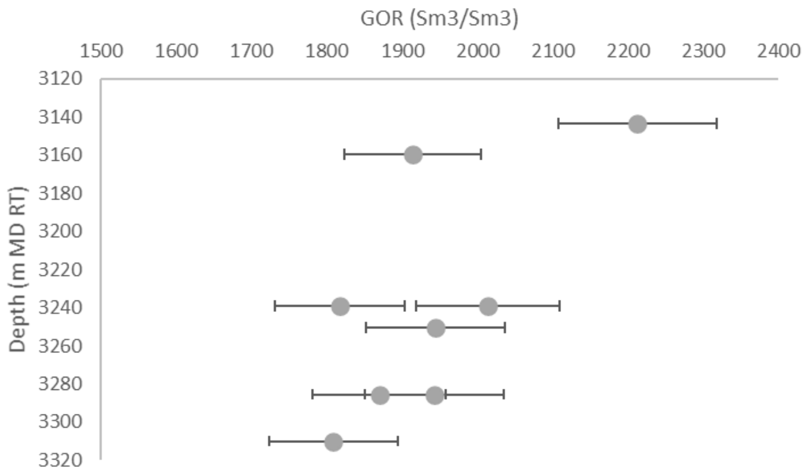
Estimated uncertainties

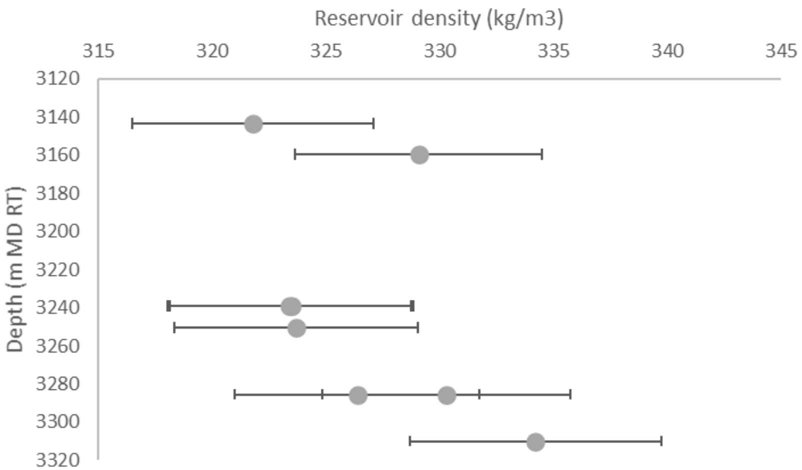






- Can have a huge impact on reservoir fluid understanding





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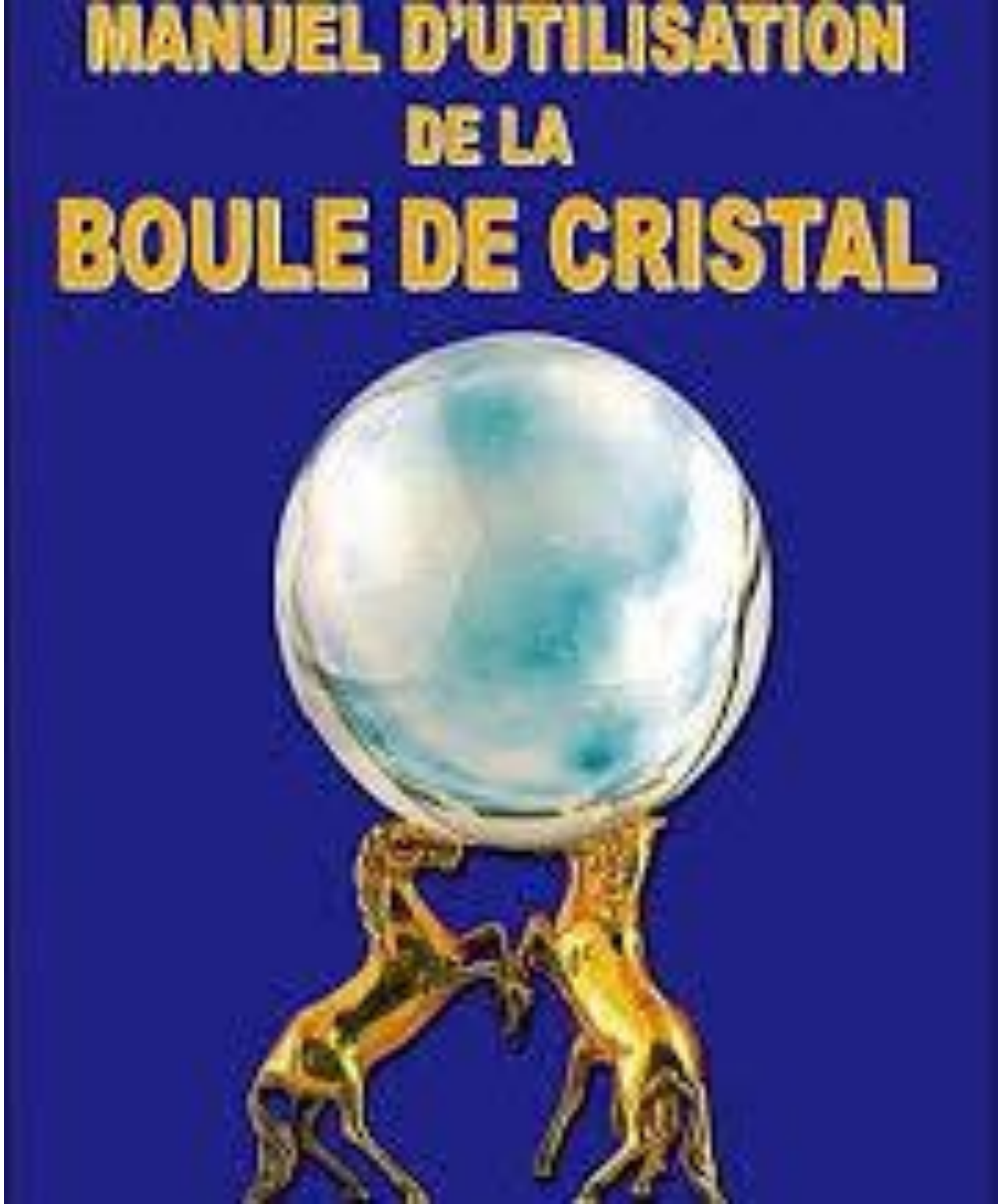
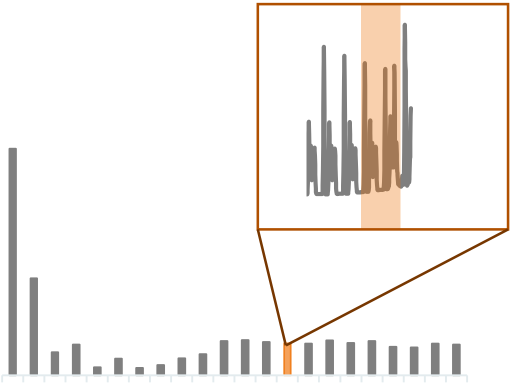
04.

Thermodynamic property correlations

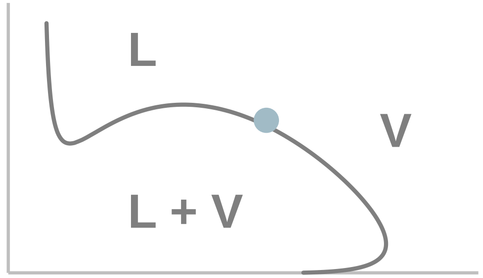


PVT properties calculations



EOS modeling

Cuts properties



Components	Mw g/mol	Reservoir fluid %mol
CO2	44.01	27.987
N2	28.01	0.468
C1	16.04	32.819
C2	30.07	4.159
C3	44.10	3.792
IC4	58.12	0.740
NC4	58.12	1.564
IC5	72.01	0.560
NC5	72.15	0.766
C6	86.00	1.070
C7	99.65	1.152
C8	113.49	1.636
C9	127.30	1.502
C10	141.10	1.279
C11	154.87	1.124
C12	168.63	1.020
C13	182.37	1.040
C14	171.35	1.022
C15	179.95	1.036
C16	187.98	0.818
C17	195.41	0.771
C18	202.25	0.847
C19	210.57	0.794
C20C29	251.49	4.603
C30C49	336.52	3.305
C50+	1063.65	4.127

Cut	Mw g/mol	Tc °C	Pc bar	Acentric factor
C6	86.00	224.49	32.74	0.30
C7	99.65	262.43	29.43	0.34
C8	113.49	293.79	26.51	0.39
C9	127.30	320.95	24.02	0.43
C10	141.10	344.70	21.87	0.48
C11	154.87	365.64	20.00	0.52
C12	168.63	384.25	18.37	0.56
C13	182.37	400.89	16.94	0.60
C14	171.35	449.25	23.56	0.49
C15	179.95	466.04	23.10	0.51
C16	187.98	481.79	22.78	0.53
C17	195.41	496.73	22.60	0.55
C18	202.25	511.05	22.56	0.56
C19	210.57	521.34	21.83	0.58
C20C29	251.49	562.52	18.52	0.69
C30C49	336.52	618.67	13.53	0.90
C50P	1063.65	677.75	7.26	1.36

17 x 4 adjustable parameters

Key issue

How to go from :

Multiple **mathematical** solutions

to

Few "EOS/physically consistent" solutions

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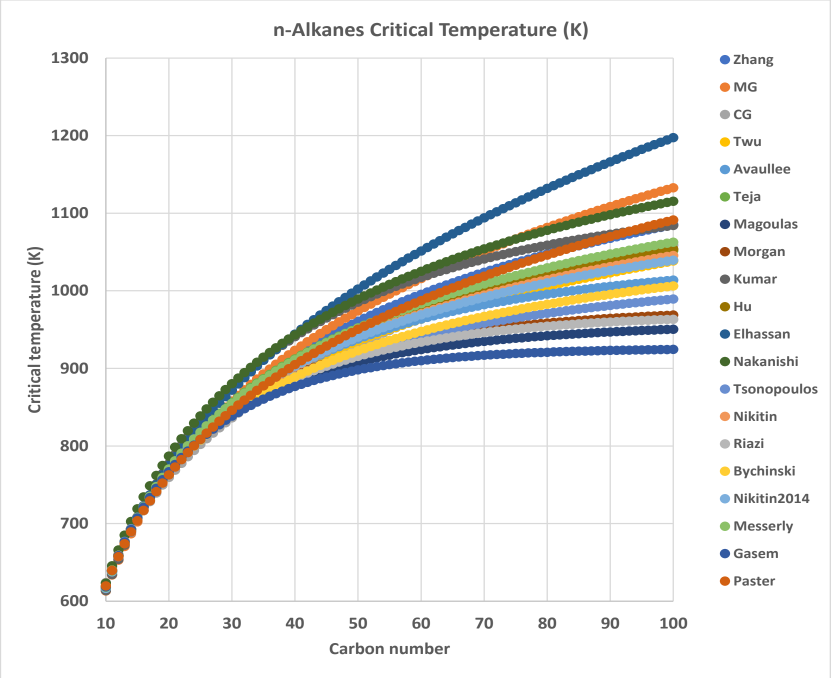
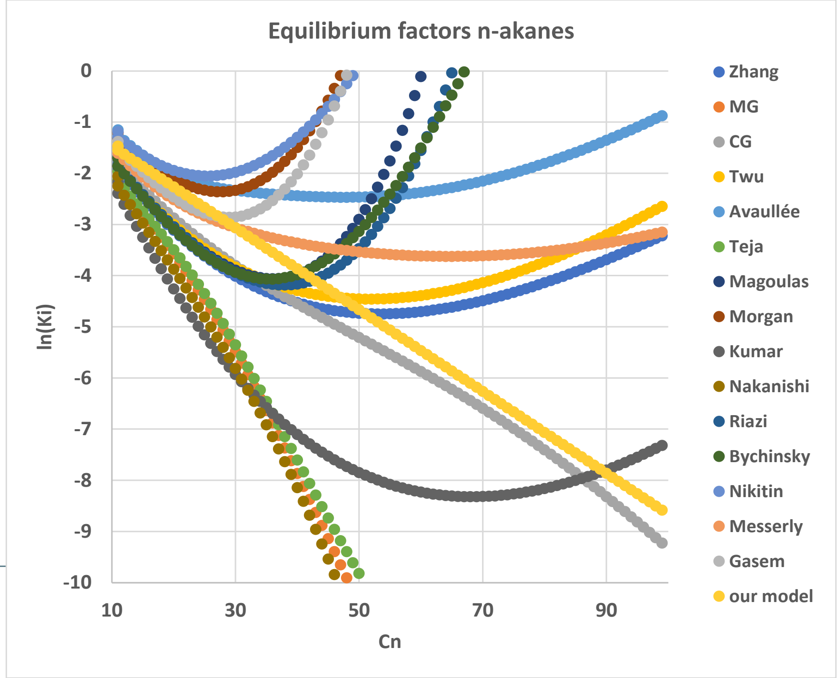
Heavy HC critical properties correlations

- Initialize EOS starting from literature correlations
  - Whitson cuts or Pedersen correlations
- Lots of discussion on behavior at very large nC
- But inconsistent K-value trend with our models
- Can be even worse using BIC



- Correlations need to be consistent with the model we are using!
- Agreement with experimental data is second order!



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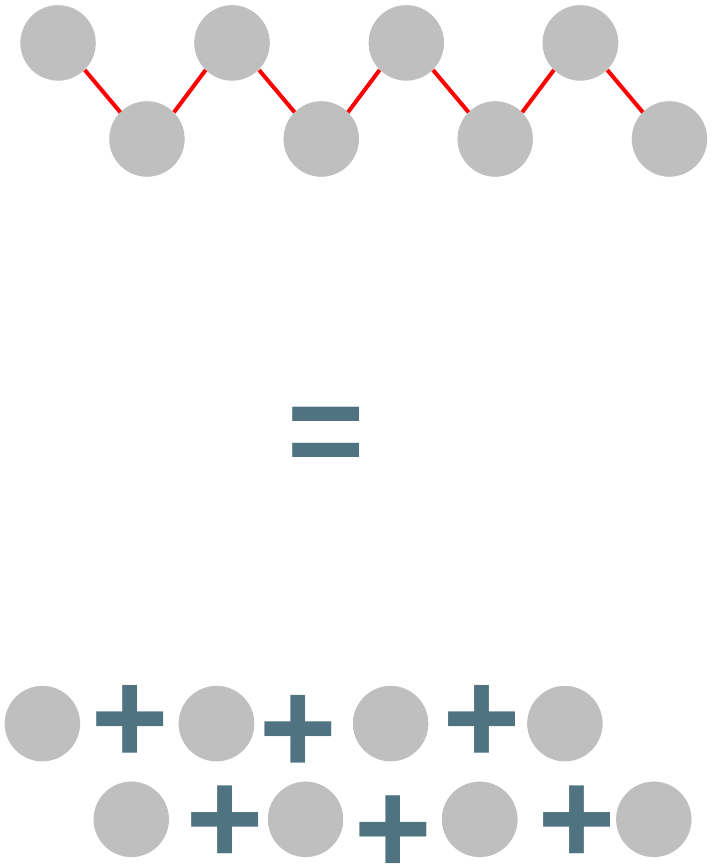
Group contribution method

- Material balance

  $N_k = \sum N_i$

- Thermodynamic

  $\mu_k = \sum \mu_i$ i.e. $\ln(\varphi_k) = \sum \ln(\varphi_i)$



Application to PR-EOS :

- $\ln(\varphi_k) = C_0 + C_1 \sum b_i + C_2 \sum (1 + m_i)\sqrt{a_{c,i}} + \sum C_3 m_i \sqrt{b_i}$
- $\ln(K_k) = \sum \Delta C_0 + \Delta C_1 \sum b_i + \Delta C_2 \sum (1 + m_i)\sqrt{a_{c,i}} + \Delta C_3 \sum m_i \sqrt{b_i}$

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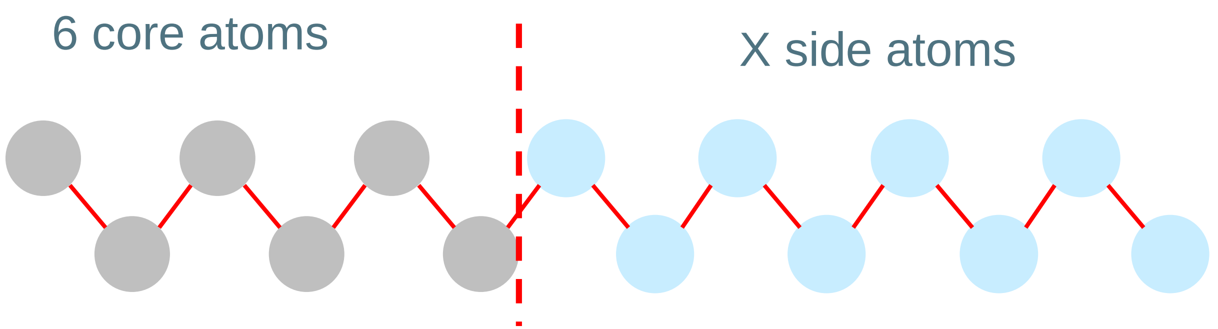
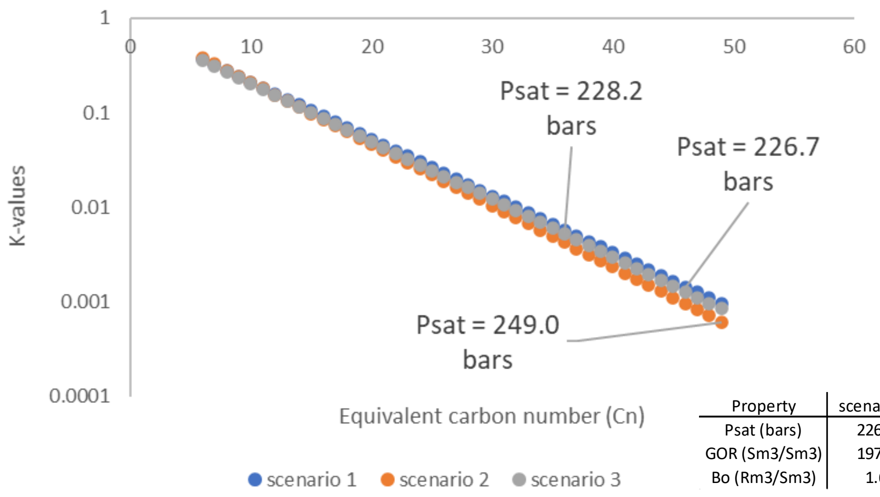
Application to real cases



Finally

- $\alpha = \sum_{i=1}^{2} n_i \frac{T_{c,i}}{P_{c,i}}$
- $m = \frac{\sum_{i=1}^{2} n_i m_i \sqrt{\frac{T_{c,i}}{P_{c,i}}}}{\sqrt{\alpha}}$
- $P_c = \left(\frac{\sum_{i=1}^{2} n_i (1+m_i) \frac{T_{c,i}}{\sqrt{P_{c,i}}}}{\alpha(1+m)} \right)^2, T_c = \alpha \times P_c$

	Core	side		
		scenario 1	scenario 2	scenario 3
m	0.303	0.262	0.255	0.230
Tc, K	159.1	97.5	102.2	92.0
Pc, bar	59.1	51.8	51.8	46.6



Property	scenario 1	scenario 2	scenario 3
Psat (bars)	226.7	249.0	228.2
GOR (Sm3/Sm3)	197.7	193.1	193.1
Bo (Rm3/Sm3)	1.6	1.6	1.6

➔ Same problem applies to BIC

Merci.