EoS for Net Zero Gases

National Gas Innovation

Phase 2 CO2

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Rev	Issue date	Description	Prep.	App.
1	03/10/2025	Issued for comment	CJ	PE
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2 Executive Summary

Equations of State (EoS) are mathematical models that describe the relationships between pressure, temperature, and volume of real gases, unlike ideal gas laws which don't account for intermolecular forces and actual volumes. EoS are used in various applications, including monitoring gas quality, modelling pipeline flow, and metering calculations for custody transfer. In metering, EoS convert measured volumes to standard units, enabling billing and network balancing in energy terms.

The AGA8 EoS is currently used by National Gas Transmission (NGT) in the calculation of density for custody transfer metering of natural gas.

This report assesses each of the EoS selected during phase 1 against experimental datasets licenced from HyCCS Tech to identify the most reliable models for different gas mixtures across relevant operating conditions. Experimental values of density for compositions with 95% CO_2 and above were extracted from the HyCCS Tech database. Limited data was available for Speed of Sound (SOS), viscosity and compressibility.

Measurement of CO_2 is complex due to the phase behaviour at typical NTS operating temperatures and pressures. National Gas are likely to be transporting CO_2 in the gaseous phase i.e. between 20-35 bar and [redacted] In this study eight different fluids were assessed as these fluids had experimental data for density within the required temperature and pressure range. The range of CO_2 purity assessed was between 95-100%.

The purity of CO_2 transported by National Gas is likely to be [redacted] with low levels of impurities but there are currently no experimental datasets available which reflect this high purity CO_2 composition. However the assessment of the most relevant gas composition i.e. 100% CO_2 shows that Span Wagner (SW) is the recommended EoS for calculating density. For fluids in this study containing CO_2 and up to 5% impurities the errors between the Span Wagner EoS and the recommended EoS are between 0.02% and 0.64% higher than the best EoS. [redacted]

Therefore Kelton recommend obtaining further experimental values for density from CO_2 mixtures with a range of impurities within the National Gas CO_2 specification as well as data for mixtures with more than two components. It would also be useful to obtain the experimental values for density across the temperature ([redacted]) and pressure (20-35 bar) range within the gaseous phase to help conclusively establish any trends.

National Gas currently calculate SOS using the AGA10[1] EoS which is not suitable for CO_2. Span Wagner and GERG2008 EoS both performed well for the 100% CO_2 experimental data at pressures of 35-70 bar however this is above the expected NTS range of 20-35 bar. Therefore it would be useful to obtain further experimental data for SOS within the required pressure range of 20-35 bar.

3 Introduction

This report assesses each of the Equations of State (EoS) selected during phase 1 against all relevant experimental datasets licenced from HyCCS Tech to identify the most reliable models for different gas mixtures across relevant operating conditions.

Experimental values of density for compositions with 95% CO2 and above were extracted from the HyCCS Tech database. Limited data was available for SOS, viscosity and compressibility.

For each mixture the following EoS were assessed:

Mixture	EoS
Pure CO2	Valderrama-Patel-Teja (VPT) [2] Span-Wagner (SW) [3]
CO_2 + impurities	AGA8[4] Peng-Robinson (PR) [5] Soave-Redlich-Kwong (SRK) [6] Valderrama-Patel-Teja (VPT) [2] Span-Wagner (SW) [3] GERG-2008 [7] Peturbed Chain – Statistical Associating Fluid Theory (PC-SAFT) [8] Simplified Cubic Plus Association (SCPA) [9] SCPA original

Table 1 Equations of State used in this study

4 Methodology

REFPROP/FloCALC software was used to calculate AGA8 and GERG-2008 EoS.
TREND software was used to calculate SRK, PR, Span-Wagner and PC SAFT EoS
HydraFLASH software was used to calculate VPT, SCPA and SCPA original EoS.

The EOS-CG values were calculated using TREND software but the results were exactly the same as the Span-Wagner EoS therefore not included in the charts.

For each composition the Relative Deviation (RD) and Average Absolute Deviation (AAD) were calculated to assess the performance of each EoS:

$$RD\rho = \frac{\rho_{calc} - \rho_{exp}}{\rho_{exp}} \times 100$$

Equation 1 Relative Deviation

$$AAD = \frac{1}{N}\sum_{i=1}^{N} |RD\rho|$$

Equation 2 Average absolute deviation

5 100% CO_2

The diagram below shows the phase envelope diagram for pure carbon dioxide (CO_2). It shows the critical point of CO_2 is close to ambient temperature. Small changes in pressure and temperature may lead to rapid changes in physical properties i.e. phase, density and compressibility.

The critical point of CO_2 is 31 °C and 73 bar therefore, at higher pressures and temperatures, CO_2 will be a supercritical fluid where it exhibits properties of both gases and liquids. National Gas are likely to be transporting CO_2 in the gaseous phase i.e. between 20-35 bar and [redacted]

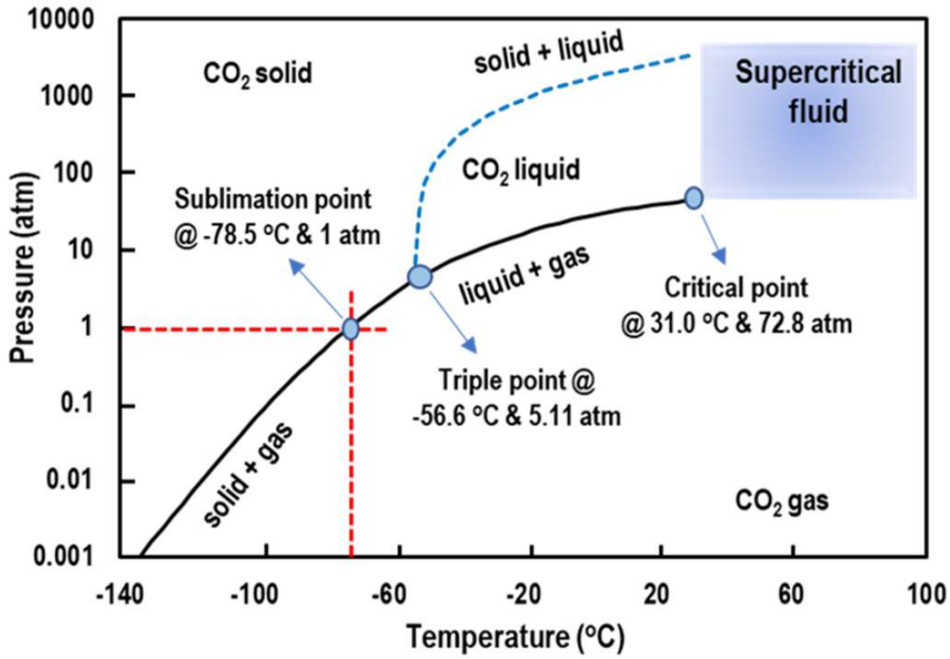

Figure 1 Reference: Measurement of CO2 Throughout the Carbon Capture and Storage (CCS) Chain

5.1 Density

Experimental values for density were compared with calculated values using Span Wagner and VPT EoS which are well known for pure CO_2. The RDρ for each EoS is plotted in the charts below over the range of 20-50 bar and the AADρ is summarised in Table 2.

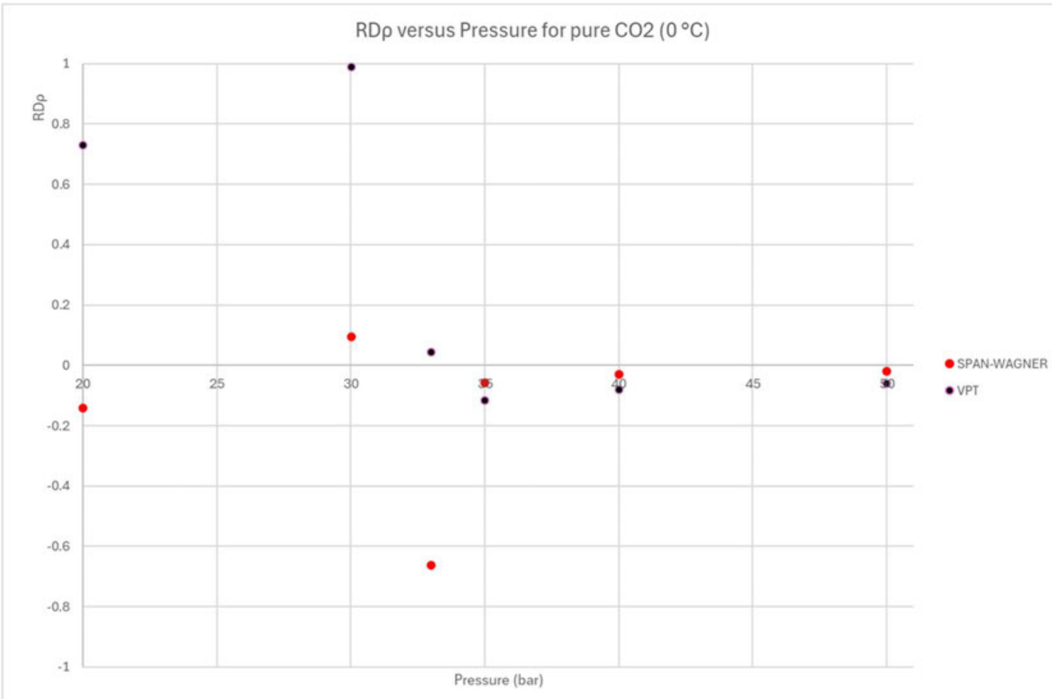

Figure 2 RDρ against pressure for pure CO2 at 0°C

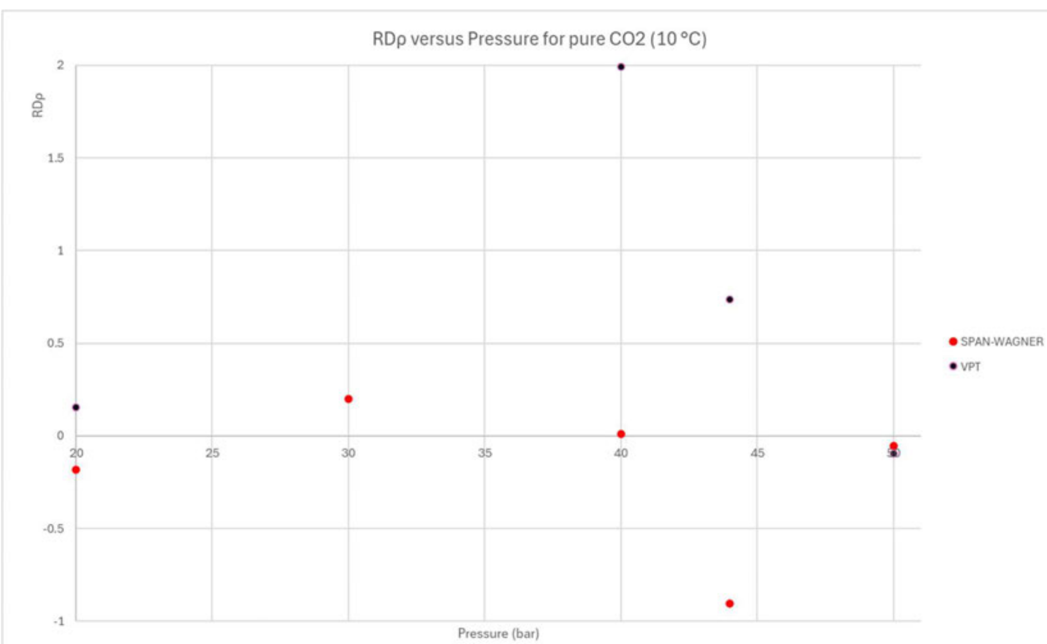

Figure 3 RDρ against pressure for pure CO2 at 10°C

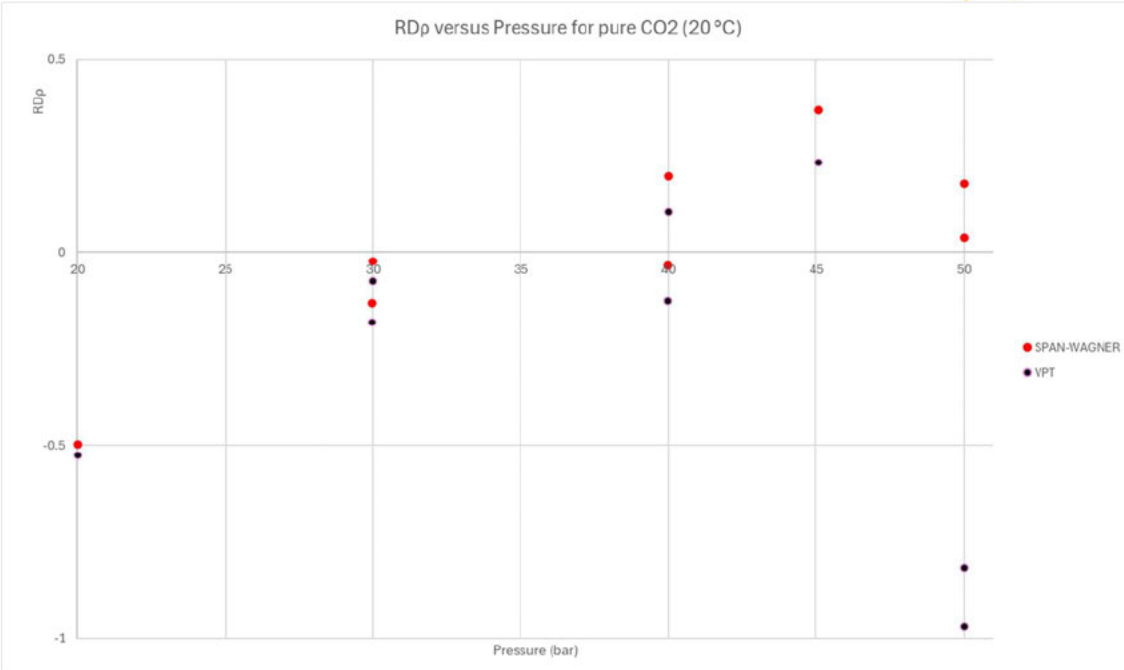

Figure 4 RDρ against pressure for pure CO2 at 20°C

	Pure CO_2 AADρ		
	0°C (20-35 bar)	**10 °C (20-35 bar)**	**20 °C (20-35 bar)**
Span-wagner	0.2387	0.1908	0.2183
VPT	0.4693	1.1365	0.2607

Table 2 Summary of AADρ for pure CO_2

The results show that Span-Wagner gives the lowest average errors (up to 0.24%) for 100% CO_2 across the pressure range of 20-35 bar and across the temperature range 0°C -20°C.

5.2 Speed of Sound

Experimental values for speed of sound (SOS) were compared with calculated values using Span Wagner and GERG2008 EoS. AGA10 is currently used for natural gas but is not suitable for pure CO_2. There was no experimental data available for NTS pressures of 20-35 bar. The RD for each EoS is plotted in the charts below over the range of 35-70 bar and the AAD is summarised in Table 3.

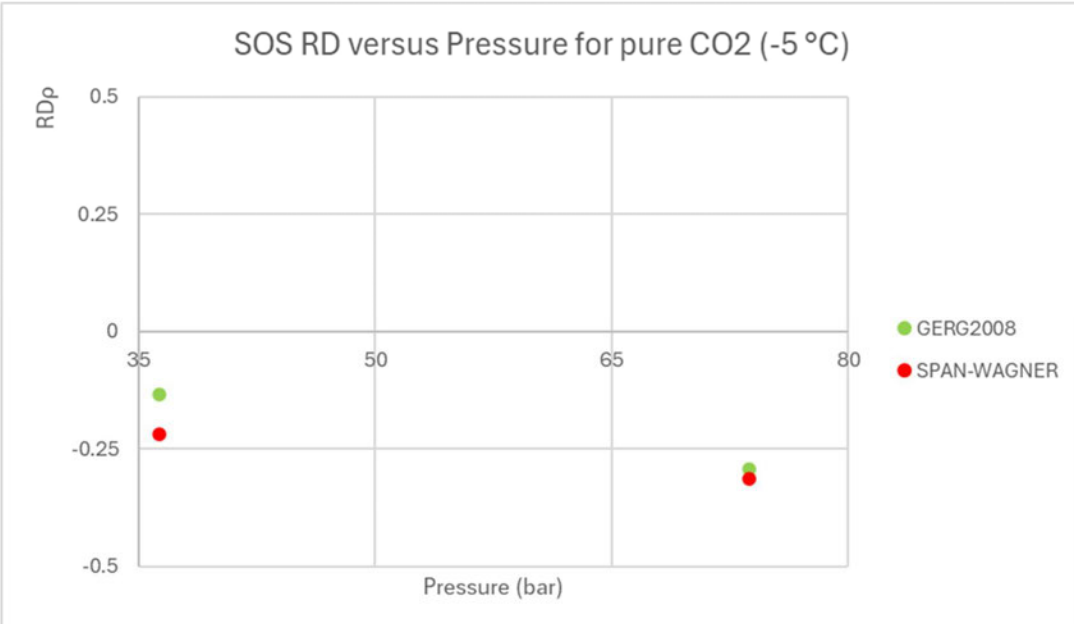

Figure 5 SOS RD against pressure for pure CO2 at -5°C

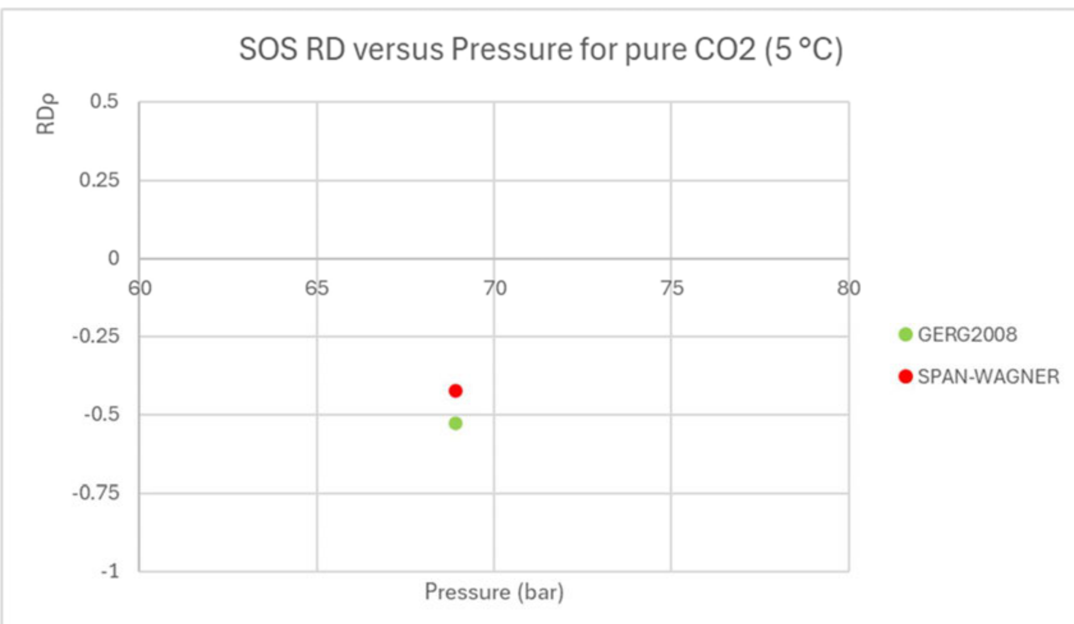

Figure 6 SOS RD against pressure for pure CO2 at 5°C

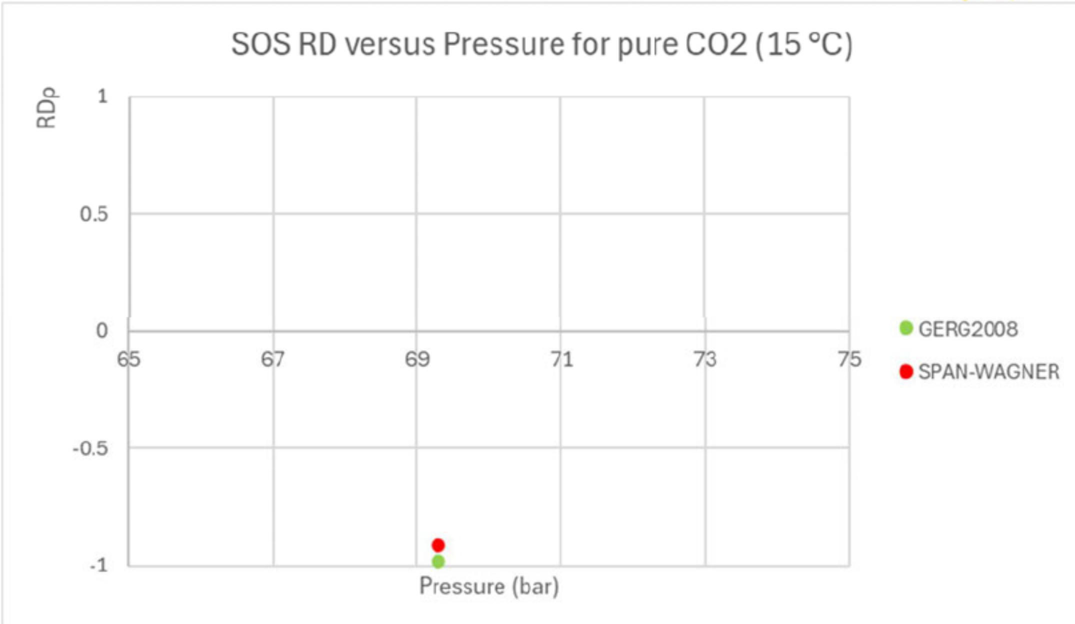

Figure 7 SOS RD against pressure for pure CO2 at 15°C

	Pure CO_2 AAD (SOS)		
	-5°C (30-70 bar)	**5 °C (30-70 bar)**	**15 °C (30-70 bar)**
Span-wagner	0.2655	0.4246	0.9126
GERG2008	0.2148	0.5288	0.9828

Table 3 Summary of SOS AAD for pure CO_2

The results show that Span-Wagner EoS gives the lowest average errors overall (up to 0.91%) for 100% CO_2 across the pressure range of 30-70 bar and across the temperature range -5°C -15°C.

6 CO_2 with impurities

A range of impurities can be in the CO_2 stream depending on the carbon capture process. The table below is provided by NPL which shows the potential contaminants:

Component	Upper limit [µmol mol^{-1}]		Notes
	Min	Max	
H_2O	20	50	
H_2S	5	20	
O_2	10	20	
CH_4	10000	40000	Combined total ≤ 4 mol %
N_2	10000	40000	
Ar	10000	40000	
H_2	50	20000	
C_2H_6	10000	40000	
C_3+	1500	20000	
CO	100	2000	
SO_x	10	100	
NO_x	10	100	
NH_3	10	1500	
Particulates	1	1	
HCl	10	70	Combined total ≤ 70 µmol mol^{-1}
HF	10	70	
HCN	10	70	
Glycol	0.025	0.05	
MEA	0.08	1	
Amine	10	10	
Formaldehyde	20	60	Combined total ≤ 60 µmol mol^{-1}
Acetaldehyde	20	60	
Cadmium	0.01	0.03	
Selexol	0.6	0.6	

Table 4 Reference: Assessment of measurement technologies for trace level impurities present in CO2 gas streams for CCUS applications, Manohara Gudiyor Veerabhadrappa, Rob Wessel, Diane Turner, Sam Bartlett And Arul Murugan

The EoS based on pure CO_2 won't be valid for CO_2 with impurities as the phase diagram will look different.

Examples of phase diagrams for CO_2 with methane and nitrogen impurities are shown in Figure 8 and Figure 9. The area under the curve is the two phase region where both gas and liquid are present. In terms of flow measurement this multiphase area should be avoided. The liquid phase would occur at lower temperatures and gaseous phase would occur at higher temperatures.

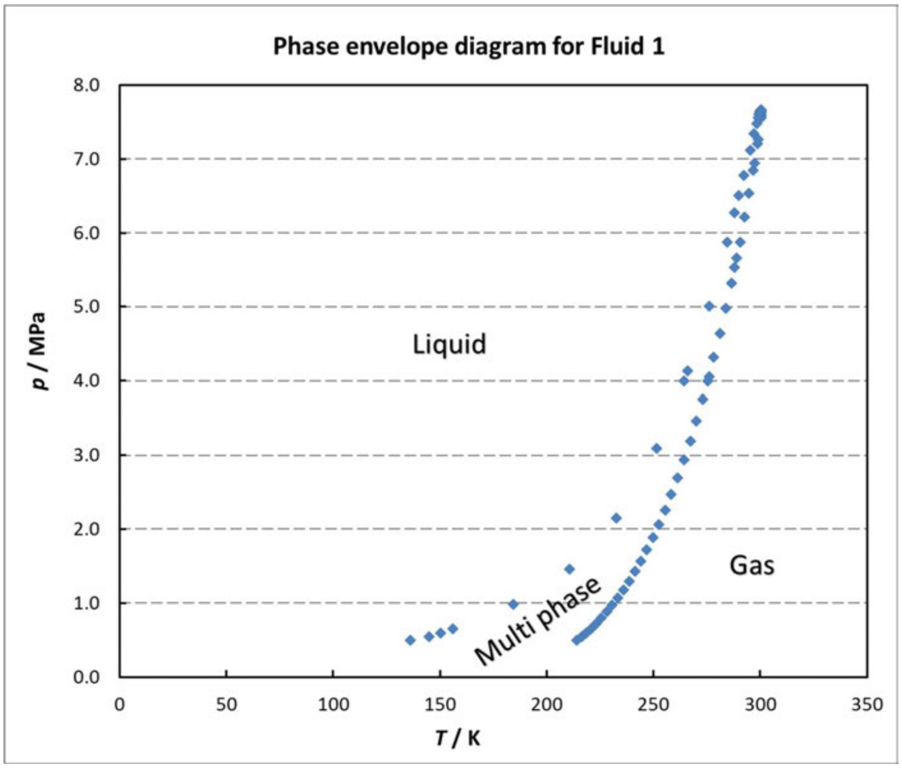

Figure 8 Phase diagram for 95%CO2 + 5% CH4

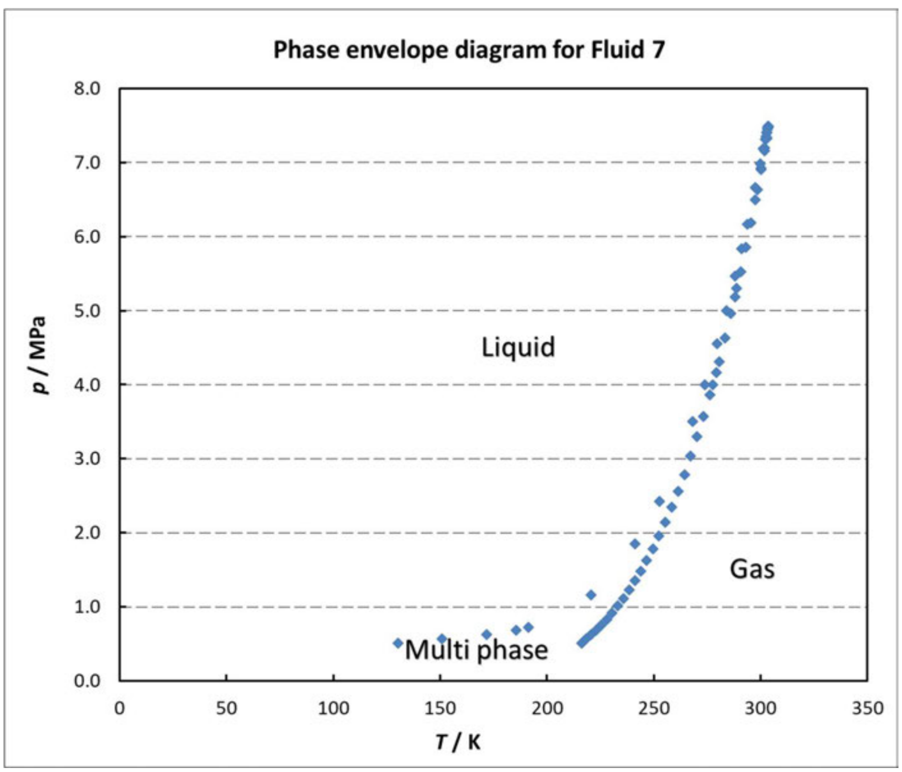

Figure 9 Phase diagram for 98.73% CO2 + 1.27% N2

6.1 Density

Experimental values for density were available for each of the compositions (mol %) in Table 5 below. Values of density (kg/m3) were then calculated using the EoS identified in Table 1.

The RDρ has been plotted for each EoS across the gaseous phase temperature range of [redacted] and pressure range of 20-50 bar in sections 6.1.1 to 6.1.7. The AAD has been derived for the NTS process conditions where possible i.e. 20-35 bar and [redacted]

Fluid	CO_2	CH_4	C_2H_6	H_2	N_2
1	95	5			
2	99.82		0.18		
3	97.54		2.46		
4	96.98		3.02		
5	97.97			2.03	
6	95.85				4.15
7	98.73				1.27

Table 5 CO2 mixtures with experimental values for density

6.1.1 Fluid 1 (95% CO_2 + 5% CH_4)

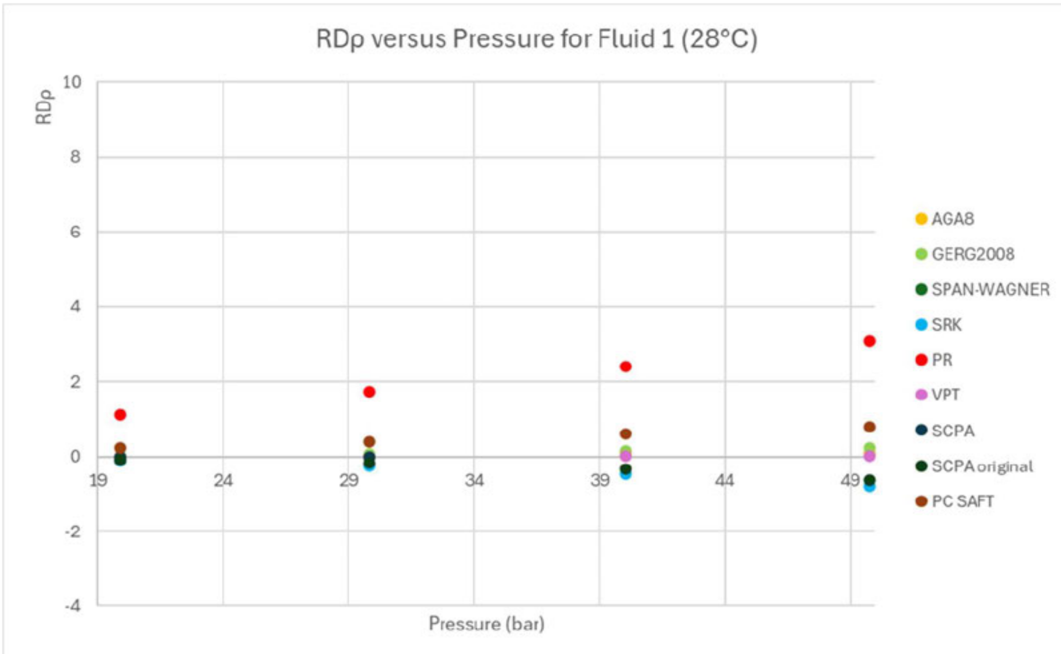

Figure 10 RDp against pressure for fluid 1 at 28°C

	Fluid 1 AADp
	28 °C (20-30 bar)
SRK	0.1914
PR	1.4187
Span-wagner	0.0508
PC SAFT	0.3195
GERG2008	0.0492
AGA8	0.0118
VPT	0.0041
SCPA Original	0.1331

Table 6 Summary of AADp for Fluid 1

VPT EoS gives the lowest average errors (0.004%) for fluid 1 across the pressure range of 20-30 bar at 28°C.

If SW EoS was used for this fluid instead of AGA8 the error would be 0.05% higher than the best EoS.

6.1.2 Fluid 2 (99.82% CO_2 + 0.18% C_2H_6)

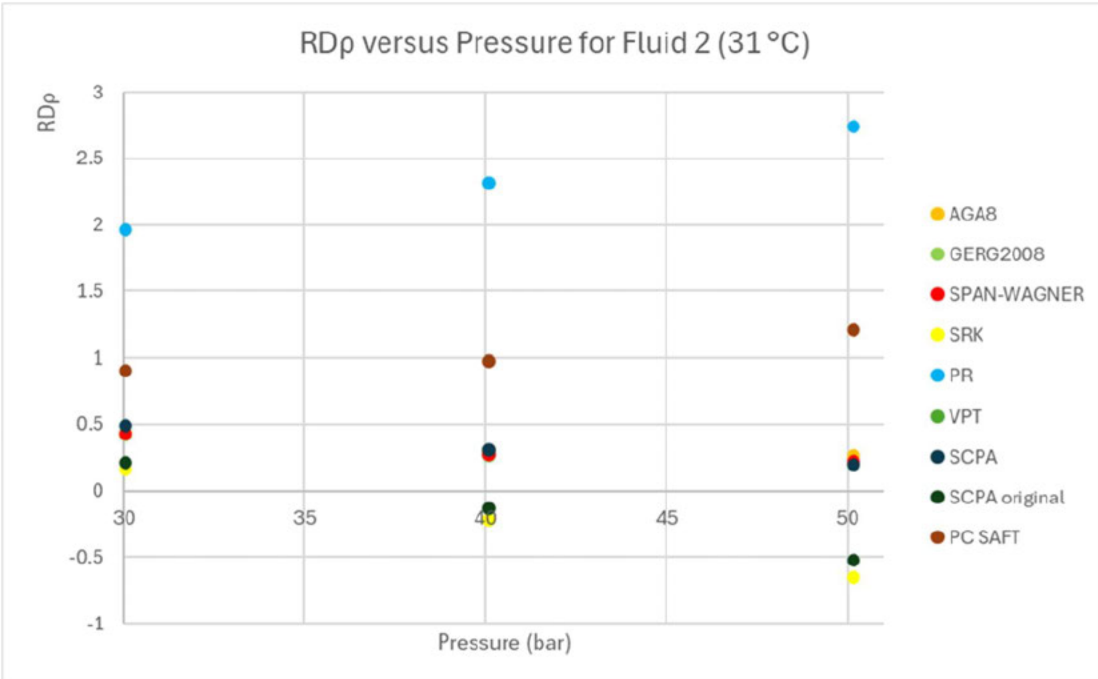

Figure 11 RDp against pressure for fluid 2 at 31°C

	Fluid 2 AADρ
	31 °C (30 bar)
SRK	0.1634
PR	1.9643
Span-wagner	0.4254
PC SAFT	0.9071
GERG2008	0.4220
AGA8	0.4375
VPT	0.3844
SCPA	0.4882
SCPA Original	0.2141

Table 7 Summary of AADp for Fluid 2

SRK gives the lowest average errors at 31 °C (0.16%) for fluid 2 at 30 bar.

If SW EoS was used for this fluid instead of VPT the error would be 0.26% higher than the best EoS.

6.1.3 Fluid 3 (97.54% CO_2 + 2.46% C_2H_6)

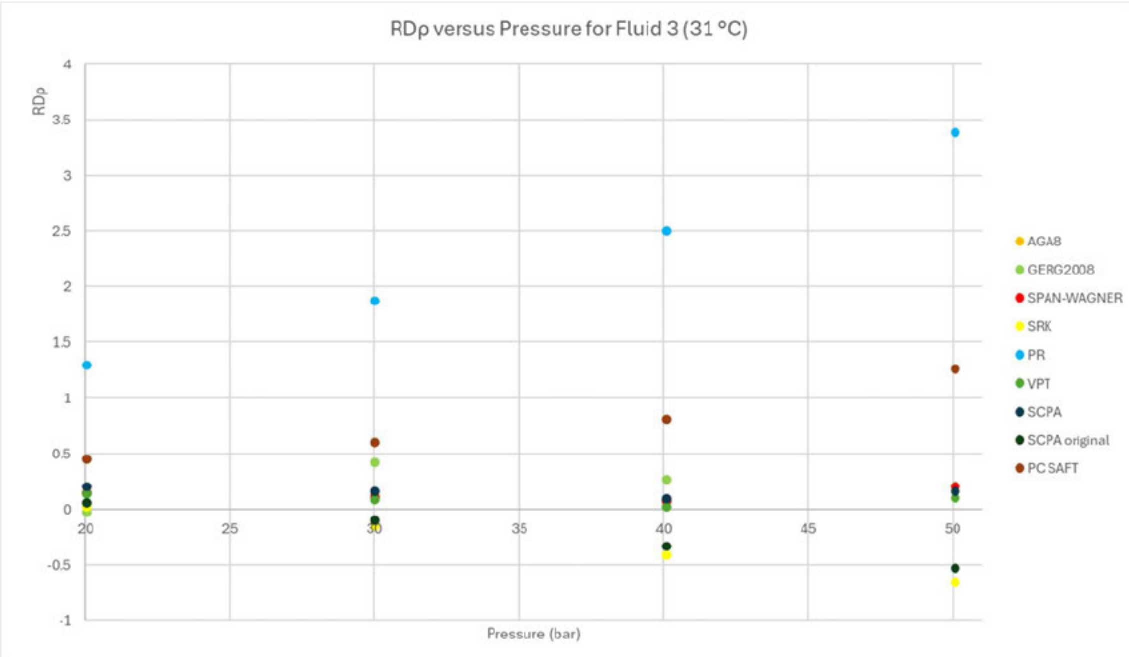

Figure 12 RDp against pressure for fluid 3 at 31°C

	Fluid 3 AADp
	31 °C (20-30 bar)
SRK	0.0887
PR	1.5837
Span-wagner	0.1258
PC SAFT	0.5273
GERG2008	0.1241
AGA8	0.1275
VPT	0.1109
SCPA	0.1836
SCPA Original	0.0779

Table 8 Summary of AADp for Fluid 3

SCPA original gives the lowest average errors at 31 °C (0.08%) for fluid 3 across the pressure range 20-30 bar.

If SW EoS was used for this fluid instead of the recommended above the errors would be 0.05% higher than the best EoS.

6.1.4 Fluid 4 (96.98% CO_2 + 3.12% C_2H_6)

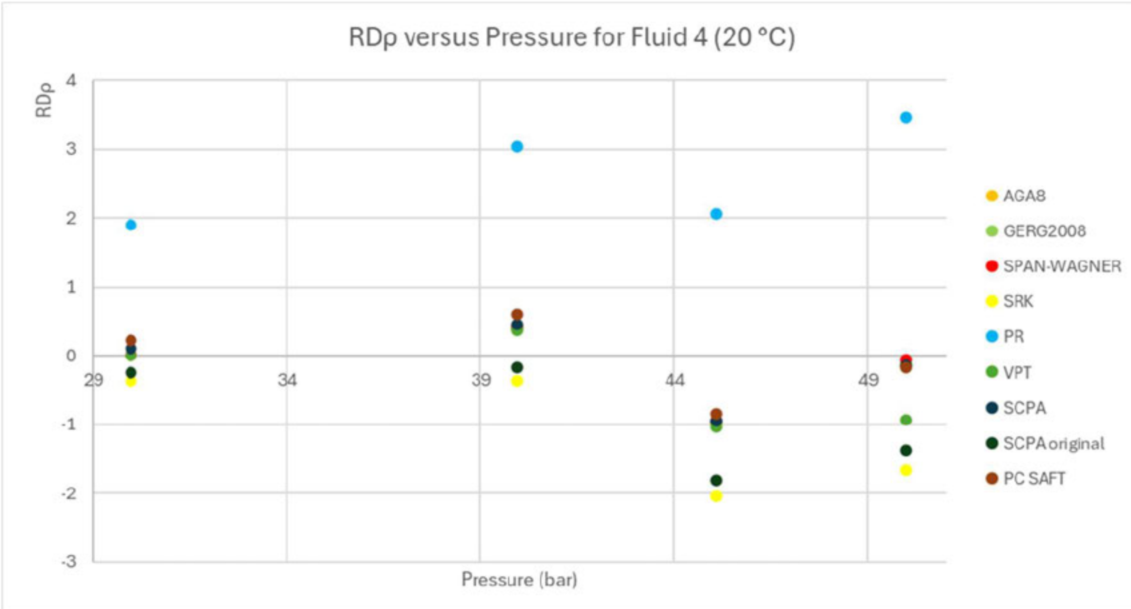

Figure 13 RDρ against pressure for fluid 4 at 20°C

	Fluid 4 AADρ
	20 °C (30 bar)
SRK	0.3641
PR	1.8956
Span-wagner	0.0218
PC SAFT	0.2277
GERG2008	0.0141
AGA8	0.0045
VPT	0.0046
SCPA	0.1100
SCPA Original	0.2522

Table 9 Summary of AADρ for Fluid 4

AGA8 EoS gives the lowest average errors (0.005%) at 20 °C for fluid 4 at 30 bar.

If SW EoS was used for this fluid instead of the recommended the errors would be 0.02% higher than the best EoS.

6.1.5 Fluid 5 (97.97% CO_2 + 2.03% H_2)

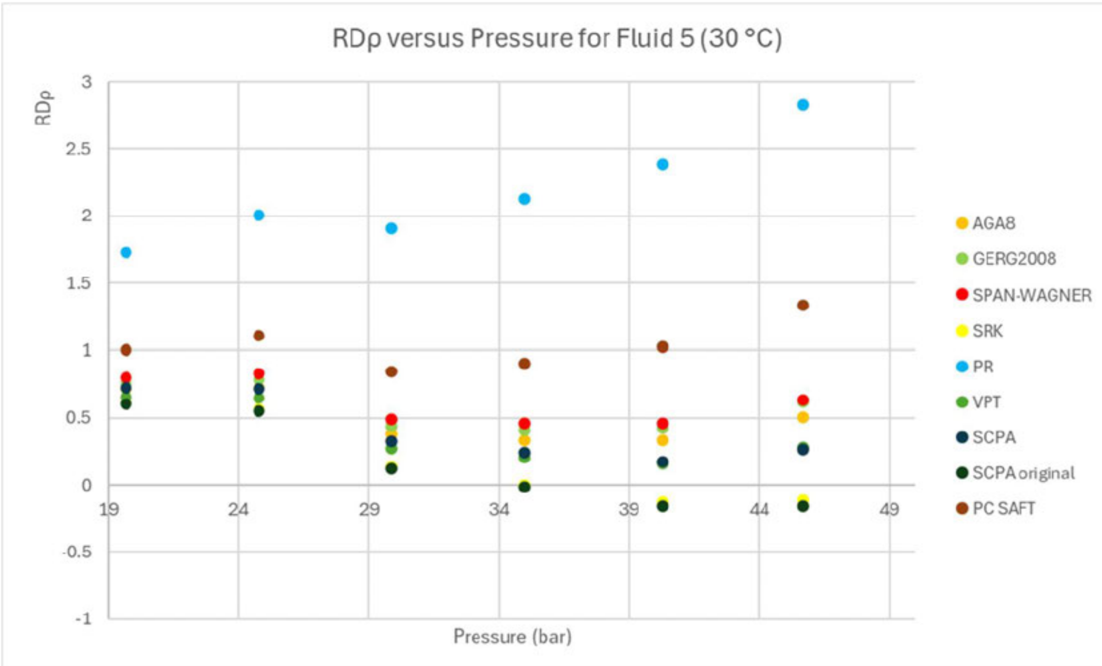

Figure 14 RDρ against pressure for fluid 5 at 30°C

	Fluid 5 AADρ
	30 °C (20-35 bar)
SRK	0.3287
PR	1.9412
Span-wagner	0.6475
PC SAFT	0.9666
GERG2008	0.5969
AGA8	0.5375
VPT	0.4460
SCPA	0.5019
SCPA Original	0.3241

Table 10 Summary of AADρ for Fluid 5

SCPA Original gives the lowest average errors at 30 °C (0.32%) for fluid 5 across the pressure range 20-35 bar.

If SW EoS was used for this fluid instead of the recommended the errors would be 0.32% higher than the best EoS.

6.1.6 Fluid 6 (95.85% CO_2 + 4.15% H_2)

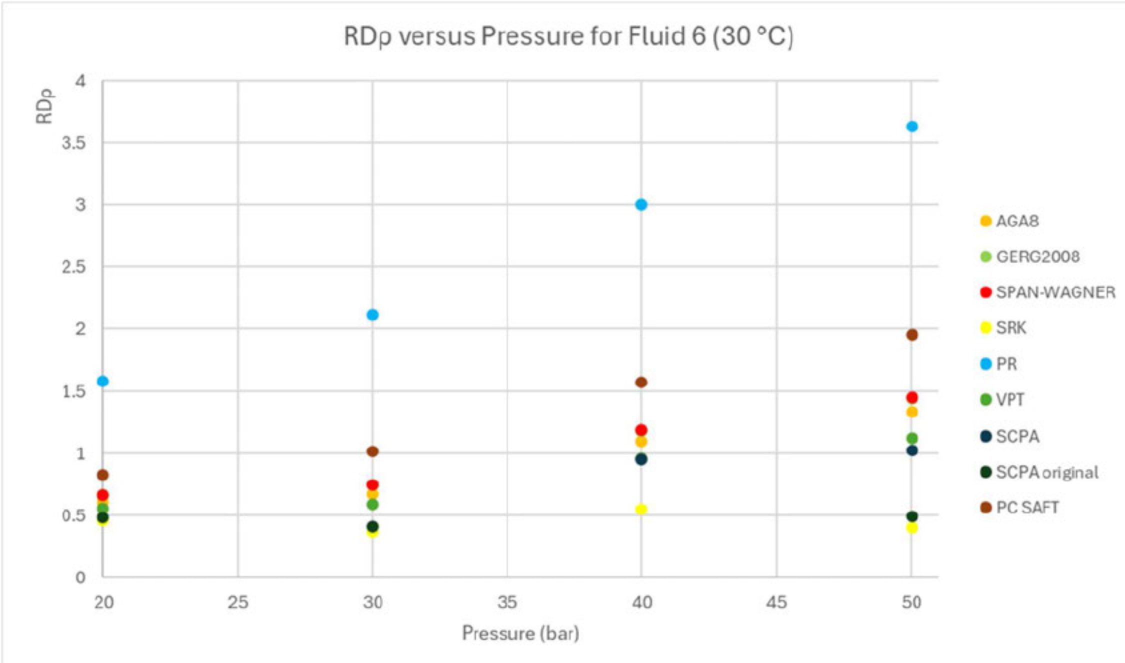

Figure 15 RDp against pressure for fluid 6 at 30°C

	Fluid 6 AADp
	30 °C (20-30 bar)
SRK	0.4133
PR	1.8497
Span-wagner	0.7051
PC SAFT	0.9226
GERG2008	0.7040
AGA8	1.2561
VPT	0.5769
SCPA Original	0.4448

Table 11 Summary of AADp for Fluid 6

SRK gives lowest average errors at 30°C (0.41%) across the pressure range 20-30 bar.

If SW EoS was used for this fluid instead of the recommended at 30°C the errors would be 0.29% higher than the best EoS.

6.1.7 Fluid 7 (98.73% CO_2 + 1.27% N_2)

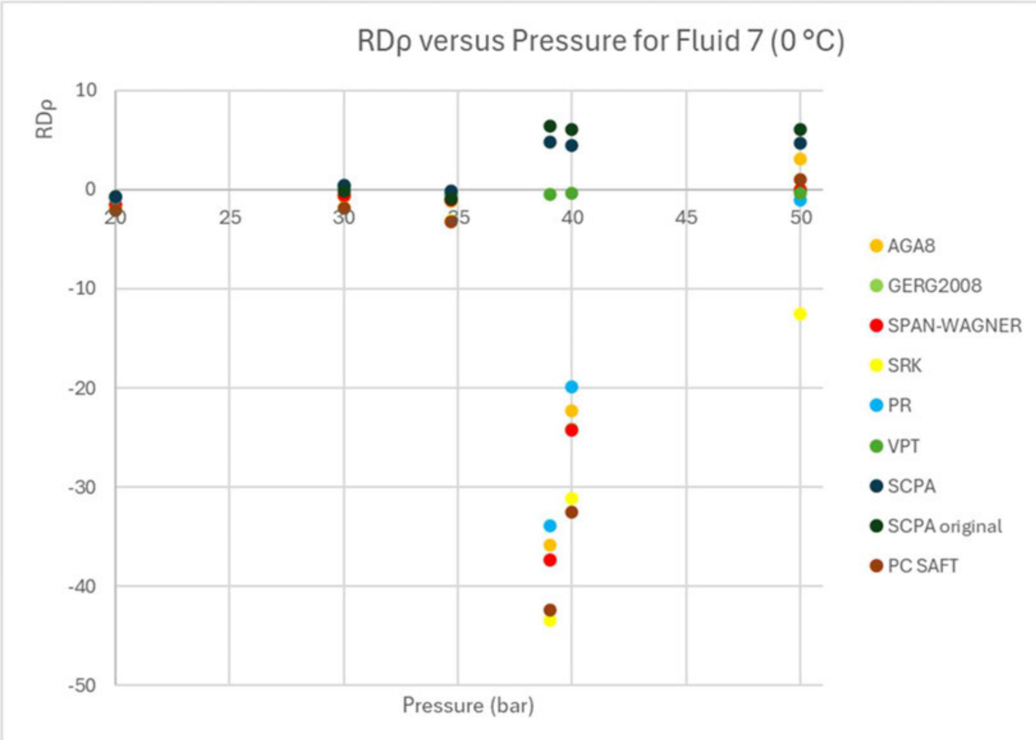

Figure 16 RDp against pressure for fluid 7 at 0°C

Figure 16 shows high errors at 40 bar due to the two phase mixture.

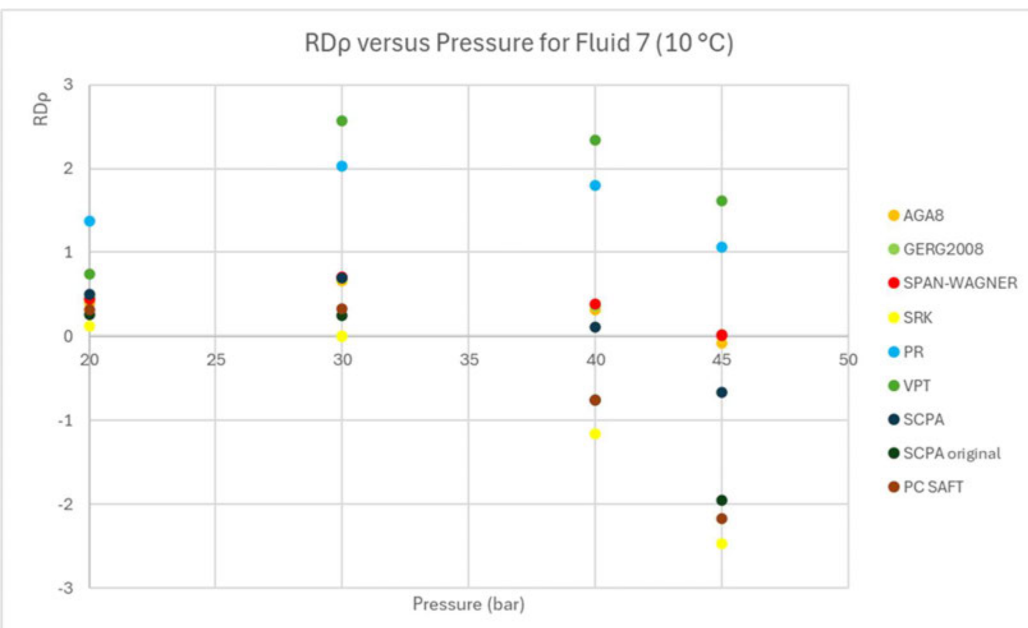

Figure 17 RDp against pressure for fluid 7 at 10°C

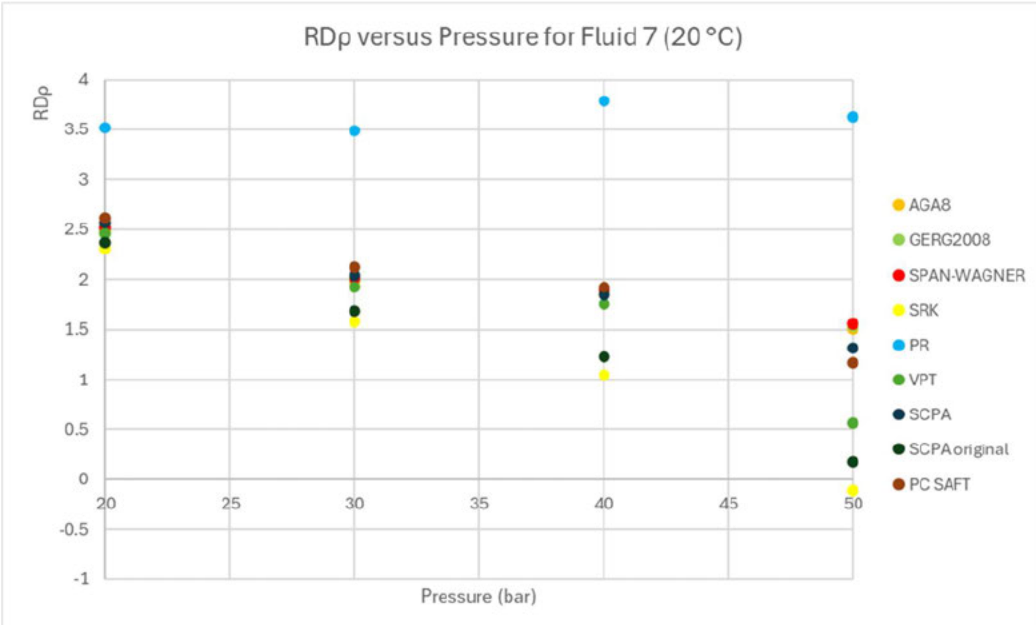

Figure 18 RDρ against pressure for fluid 7 at 20°C

Excluding the results from the two phase region gives the following errors in Table 12.

	Fluid 7 AADρ		
	0 °C (20-30 bar)	**10 °C (20-30 bar)**	**20 °C (20-30 bar)**
SRK	2.3479	0.0651	1.9377
PR	0.5218	1.6990	3.5026
Span-wagner	1.0890	0.5750	2.2637
PC SAFT	2.4044	0.3171	2.3691
GERG2008	1.1006	0.5672	2.2605
AGA8	1.1434	0.5275	2.2314
VPT	0.5192	1.6595	2.1915
SCPA	0.4501	0.5959	2.3030
SCPA Original	0.5314	0.2559	2.0274

Table 12 Summary of AADρ for Fluid 7

SCPA EoS gives lowest average errors at 0°C (0.45%), SRK gives the lowest average errors at 10°C (0.07%) , SRK give lowest errors at 20°C (1.94%) across the pressure range 20-30 bar.

If SW EoS was used for this fluid instead of the recommended the errors would be between 0.33% and 0.64% higher than the best EoS.

7 Summary

7.1 Density

Based on the AADρ for each fluid at typical NTS pressures (20-35 bar) the EoS with the lowest uncertainty for each fluid is shown in Table 13. The deviation (improved errors) between the recommended EoS and the SW EoS is also included for each fluid in the table below.

Fluid	0°C	10°C	20°C	28°C	30°C
100% CO_2	SW	SW	SW		
1 (95% CO_2 + 5% CH_4)				VPT (0.05%)	
2 (99.8% CO_2 + 0.18% C_2H_6)					SRK (0.26%)
3 (97.54% CO_2 + 2.46% C_2H_6)					SCPA original (0.05%)
4 (96.98% CO_2 + 3.02% C_2H_6)			AGA8 (0.02%)		
5 (97.97% CO_2 + 2.03% H_2)					SCPA original (0.32%)
6 (95.85% CO_2 + 4.15% N_2)					SRK (0.29%)
7 (98.73% CO_2 + 1.27% N_2)	SCPA (0.64%)	SRK (0.51%)	SRK (0.33%)		

Table 13 Summary of recommended EoS for each fluid

[redacted]

The deviations between the SW EoS and the recommended EoS for each of the other seven fluids assessed in Table 13 are between 0.02% and 0.64%.

7.2 Speed of Sound

[redacted]

7.3 Gaps in data

The range of CO_2 compositions with impurities which had experimental values for density available within the NTS temperature [redacted] and pressure (20-35 bar) range are summarised in Table 14 below:

Component	Mol %
CO_2	95-100
CH_4	5
C_2H_6	0.18-3.02
H_2	2.03
N_2	1.27-4.15%

Table 14 Range of components

[redacted]

Therefore Kelton recommend obtaining further experimental values for density from CO_2 mixtures with a range of impurities as shown in Table 15 as well as data for mixtures with more than two components. It would also be useful to obtain the experimental values for density across the relevant pressure (20-35 bar) and temperature [redacted] range to help conclusively establish any trends.

[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]

[redacted] *Recommended range of impurities*

Additional experimental datasets would also be useful for speed of sound, viscosity and compressibility at the required NTS process conditions.

8 References

1	AGA Report No.10 – Natural Gas Speed of Sound
2	Valderrama, J. O., 1990, A Generalized Patel-Teja Equation of State for Polar and Non-Polar Fluids and Their Mixtures, J. Chem. Eng Japan
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5	Peng, D.-Y.; Robinson, D. B. (1976): A New Two-Constant Equation of State, Ind. Eng. Chem. Fundam., 15(1), 59 - 64.
6	Soave, G. (1972): Equilibrium Constants from a Modified Redlich-Kwong Equation of State. Chem. Eng. Sci. 27, 1197 - 1203.
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8	Gross, J.; Sadowski, G. (2001): Perturbed-Chain SAFT: An Equation of State Based on a Perturbation Theory for Chain Molecules. Ind. Eng. Chem. Res. 40(4), 1244 - 1260.
9	Citation (APA): Velho, P., Liang, X., Macedo, E. A., Gómez, E., & Kontogeorgis, G. M. (2021). Towards a predictive Cubic Plus Association equation of state. Fluid Phase Equilibria, 540, Article 113045

EoS for Net Zero Gases

National Gas Innovation

Phase 2 H2

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Contents

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The AGA8 EoS is currently used by National Gas Transmission (NGT) in the calculation of density for custody transfer metering of natural gas.

This report assesses each of the EoS selected during phase 1 against experimental datasets licenced from HyCCS Tech to identify the most reliable models for different gas mixtures across relevant operating conditions. The study focused on three types of mixtures: hydrogen with impurities (>85% H_2), hydrogen blends with natural gas (≤20 % H_2) and binary mixtures with hydrogen (≤20 % H_2). The gas properties considered include density, speed of sound, viscosity, and the isentropic exponent. Density was selected as the primary property examined in this study due to its critical role in precise metering and the relatively greater availability of experimental data compared to other gas properties.

For pure hydrogen, GERG, Span–Wagner, and AGA 8 EoS all performed well, with Span–Wagner most accurate below 0 °C and AGA 8 between 0–50 °C. In high-H_2 binary mixtures, AGA 8 outperformed others for hydrogen–propane (>95% H_2). Peng-Robinson (PR) performed best for hydrogen–nitrogen (90% H_2), while Peng-Robinson (PR) was superior at 23 °C for hydrogen–methane (85% H_2), with PC-SAFT performing better at 27 °C. Limited data in these mixtures highlight the need for further experimental validation.

Looking at the analysis for H_2 blends (≤20 % H_2), the data shows that all EoS (GERG, Span–Wagner, and REFPROP) perform similarly within 20 % H_2 blends. AGA 8 is generally accurate at 0°C and 50°C while GERG performs best at mid-range temperatures 20°C, and Span–Wagner at low temperatures in CH_4-dominated mixtures. These results provide guidance for selecting suitable EoS models for hydrogen-blended natural gas across varying compositions, pressures, and temperatures.

Mixture	Temperature	REFPROP			GERG			AGA 8		
		50	70	AADp	50	70	AADp	50	70	AADp
NG	0°C	0.056	0.062	**0.059**	0.053	0.062	**0.058**	0.086	0.087	**0.087**
	20°C	0.015	0.049	**0.032**	0.013	0.046	**0.029**	0.039	0.073	**0.056**
	50°C	0.026	0.053	**0.040**	0.021	0.049	**0.035**	0.041	0.074	**0.058**
3%	0°C	0.014	0.067	**0.040**	0.006	0.058	**0.032**	0.035	0.070	**0.053**
	20°C	0.113	0.103	**0.108**	0.106	0.093	**0.100**	0.127	0.109	**0.118**
	50°C	0.116	0.094	**0.105**	0.110	0.086	**0.098**	0.124	0.100	**0.112**
10%	0°C	-0.009	0.019	**0.014**	-0.024	-0.005	**0.015**	0.018	0.019	**0.018**
	20°C	0.034	0.079	**0.057**	0.024	0.061	**0.043**	0.049	0.077	**0.063**
	50°C	-0.014	0.007	**0.010**	-0.019	-0.003	**0.011**	-0.008	0.004	**0.006**
15%	0°C	-0.099	-0.069	**0.084**	-0.115	-0.096	**0.105**	-0.072	-0.069	**0.070**
	20°C	0.064	0.044	**0.054**	0.055	0.026	**0.040**	0.077	0.039	**0.058**
	50°C	-0.097	-0.083	**0.090**	-0.099	-0.092	**0.095**	-0.092	-0.090	**0.091**
20%	0°C	-0.061	-0.038	**0.050**	-0.073	-0.063	**0.068**	-0.026	-0.029	**0.027**
	20°C	0.000	0.013	**0.007**	-0.005	-0.002	**0.004**	0.019	0.015	**0.017**
	50°C	-0.066	-0.066	**0.066**	-0.065	-0.071	**0.068**	-0.057	-0.067	**0.062**

Table 1 EoS models perfermance across NG and Blends with up to 20% H_2

The table above compiles data for natural gas with hydrogen content ranging from 0% to 20%, showing the AAD across the NTS pressure (50–70 bar) at temperatures of 0°C, 20°C, and 50°C. It allows comparison of the performance of different EoS models at these conditions.

The chart below highlights AGA 8, the current standard for density calculations in custody transfer systems, across varying H_2 blends. The following chart illustrates the performance of GERG with NG and the different H_2 blends.

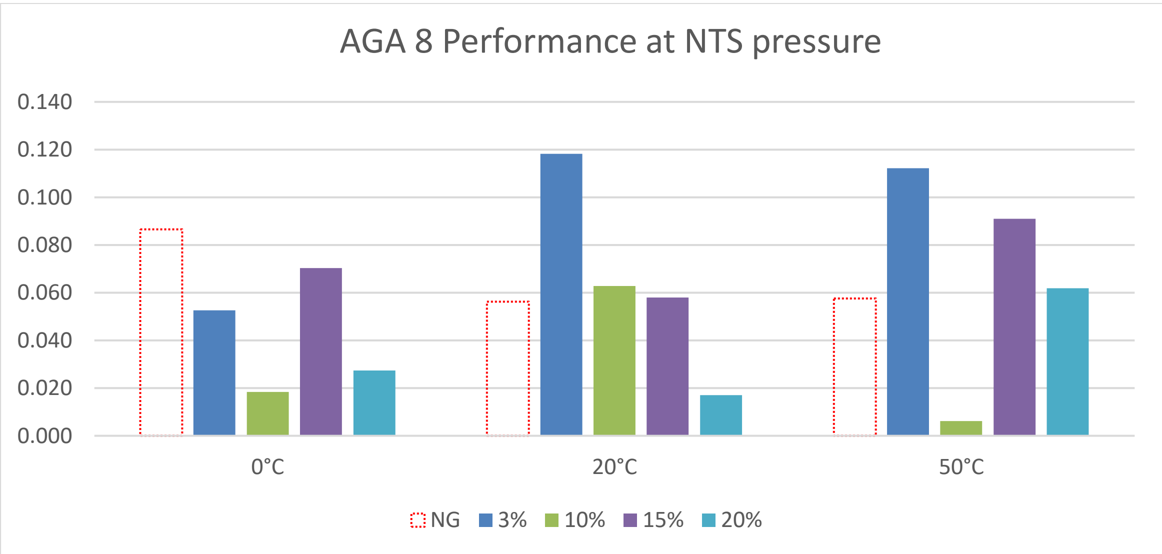

Figure 1 AGA 8 performance across NG and different H_2 blends at NTS pressure

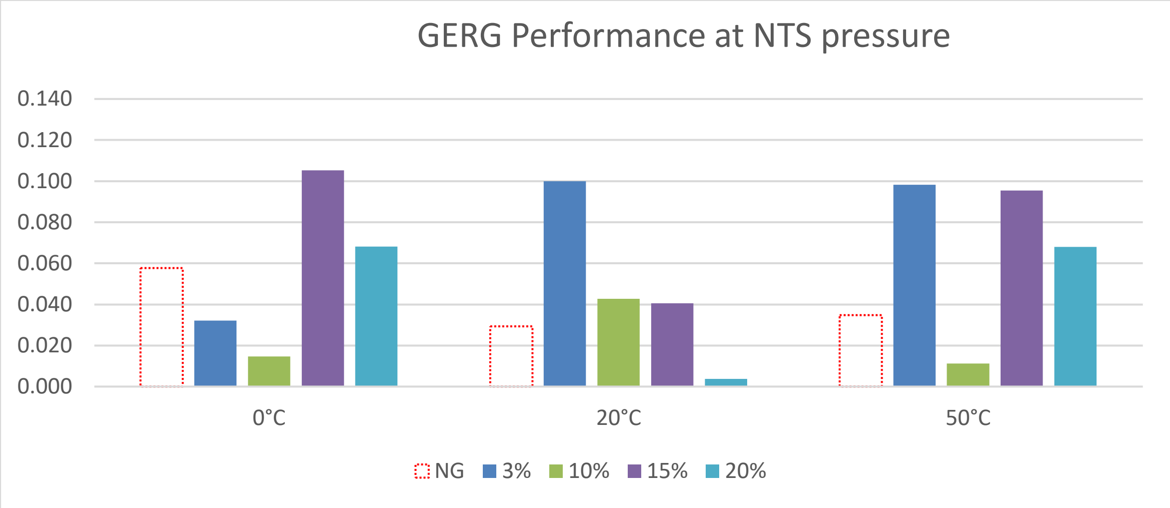

Figure 2 GERG performance across NG and different H_2 blends at NTS pressure

3 Introduction

This report assesses each of the Equations of State (EoS) selected during phase 1 against experimental datasets licenced from HyCCS Tech to identify the most reliable models for different gas mixtures across relevant operating conditions.

The majority of the experimental data was for density with limited information for SOS, viscosity and compressibility. Experimental values (density, SOS, viscosity and Z) for compositions within the following range were extracted from the HyCCS Tech database:

- Hydrogen plus impurities (90% hydrogen and above)
- Hydrogen blends (up to 20% hydrogen in natural gas)

For each mixture the following EoS were assessed:

Mixture	EoS
NG + H_2 blends	AGA8[1] GERG-2008[2] REFPROP[3]
Binary – mixture with up to 20 % H_2	AGA8 GERG-2008 REFPROP Span -Wagner[4] Peng-Robinson (PR)[5] Soave-Redlich-Kwong (SRK) [6] PC-SAFT[7]
H_2 + impurities	AGA8 Peng-Robinson (PR) Soave-Redlich-Kwong (SRK) GERG-2008 Span–Wagner

Table 2 Equations of state used in this study

4 Methodology

REFPROP/FloCALC software was used to calculate REFPROP-default, AGA8 and GERG-2008 EoS. TREND software was used to calculate SRK, PR, Span-wagner and PC SAFT EoS.

REFPROP-default and GERG-2008 differ in how they handle mixtures. REFPROP-default uses default mixing rules for pure-component Helmholtz equations, which may not be fully optimized for hydrogen–natural gas blends. GERG-2008, however, includes fitted interaction parameters for natural gas mixtures, yielding more consistent density and compressibility predictions, especially at higher hydrogen fractions and pressures.

For each fluid mixture the Relative Deviation (RD) and Average Absolute Deviation (AAD) were calculated to assess the performance of each EoS:

$$RD\rho = \frac{\rho_{calc} - \rho_{exp}}{\rho_{exp}} \times 100$$

Equation 1 Relative Deviation

$$AAD = \frac{1}{N}\sum_{i=1}^{N} |RD\rho|$$

Equation 2 Average Absolute Deviation

5 Scope of Analysis

This report focuses on hydrogen-rich mixtures containing more than 90% H_2 with impurities, as well as hydrogen–natural gas blends with up to 20% H_2. Density was the primary parameter assessed, given its importance on flow calculations and the availability of the most complete dataset, while speed of sound, viscosity, and compressibility factor were evaluated where experimental data allowed.

Model performance was measured using relative deviation (RD) and average absolute deviation (AAD) across the available pressures and temperatures. Based on KELTON's experience and depending on the experimental dataset's availability, the dataset was filtered for gas mixtures in an attempt to cover the range of at least –10 °C to 40 °C and 0–80 bar where applicable. However, this requirement was not fulfilled in all mixtures.

A more detailed analysis was undertaken for both pure hydrogen (100% H_2) in section 6.1.1 and low-level hydrogen blends (3% % H_2 in natural gas) in section 7.1.1. This approach ensures that the study captures both the near-term operational scenarios where small hydrogen fractions are expected to be introduced into the network, as well as the longer-term strategic ambition of transitioning to a fully hydrogen-based system.

All other studied fluids were analysed by plotting the relative deviation (RD) against pressure at each temperature. For every temperature set, the average absolute deviation (AAD) was calculated to quantify the overall error of each EoS. These results were consolidated into a discussion section highlighting the availability of the experimental datasets, the relative performance of the EoS models, identifying the conditions under which each EoS is most reliable and where their limitations become apparent.

6 Hydrogen (H_2) with impurities

6.1 Density

Fluid	H2	CH4	C3H8	N2
1	1			
2	0.95003		0.04997	
3	0.8587	0.1413		
4	0.9039			0.0961

Table 3 Composition used for hydrogen with impurities mixtures density calculations

Note: Best EoS performance is highlighted in green.

6.1.1 Fluid 1 (100% H_2)

Temperature -75°C

Pressure (bar)	Span Wagner	GERG	PR	SRK	AGA 8
4.04	0.706	0.714	0.942	0.773	0.682
10.12	0.009	0.026	0.582	0.170	-0.049
20.24	0.096	0.121	1.200	0.398	-0.016
40.49	-0.043	-0.014	2.005	0.490	-0.242
101.14	0.011	0.046	4.163	0.963	-0.286
202.41	-0.062	0.041	5.970	1.022	-0.141
303.47	-0.034	0.089	6.733	0.774	0.154
404.59	-0.014	0.075	6.915	0.319	0.269
505.83	0.009	0.055	6.804	-0.223	0.351
AADp	**0.109**	0.131	3.924	0.570	0.243

Table 4: Fluid 1 RDp and AADp for each EoS at -75°C

Since PR and SRK are clearly less accurate once compared against the experimental data, the chart below does not include PR and SRK to focus on the accuracy of the other EoS examined in this study.

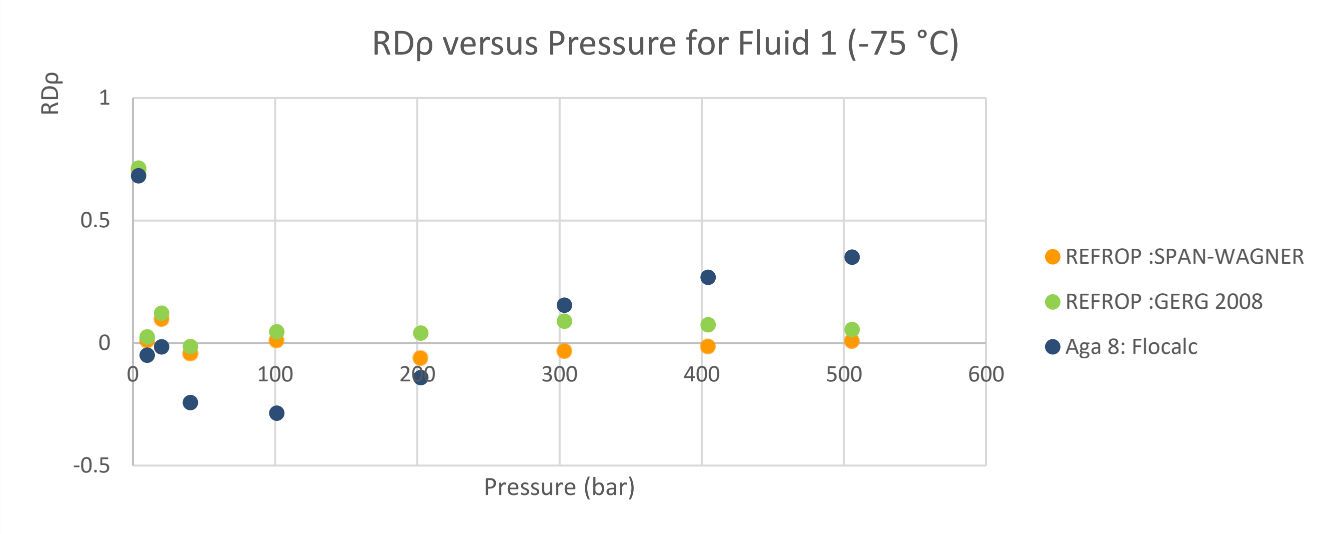

Figure 3: RDρ versus Pressure for Fluid 1 (-75 °C)

Data analysis at -75°C

- Span–Wagner and GERG are the most reliable EOS at –75 °C. Especially at pressures higher than 10 bar.
- PR is unsuitable in this condition due to extreme overestimation.
- SRK performs moderately but still drifts at higher pressure.
- AGA 8 provides a balance but cannot match Span–Wagner/GERG precision.

Temperature -50 °C

Pressure (bar)	Span Wagner	GERG	PR	SRK	AGA 8
4.06	-0.087	-0.081	0.109	-0.034	-0.100
10.13	0.252	0.264	0.734	0.380	0.221
20.25	0.007	0.027	0.937	0.248	-0.052
40.46	-0.060	-0.037	1.676	0.368	-0.165
101.09	0.037	0.056	3.629	0.819	-0.119
202.33	-0.044	0.016	5.330	0.875	-0.073
303.53	-0.044	0.045	6.132	0.666	0.084
404.63	-0.023	0.052	6.414	0.284	0.106
505.88	0.001	0.045	6.397	-0.196	0.017
AADρ	0.062	0.069	3.484	0.430	0.104

Table 5: Fluid 1 RDρ and AADρ for each EoS at -50°C

Since PR and SRK are clearly less accurate once compared against the experimental data, the chart below does not include PR and SRK to focus on the accuracy of the other EoS examined in this study.

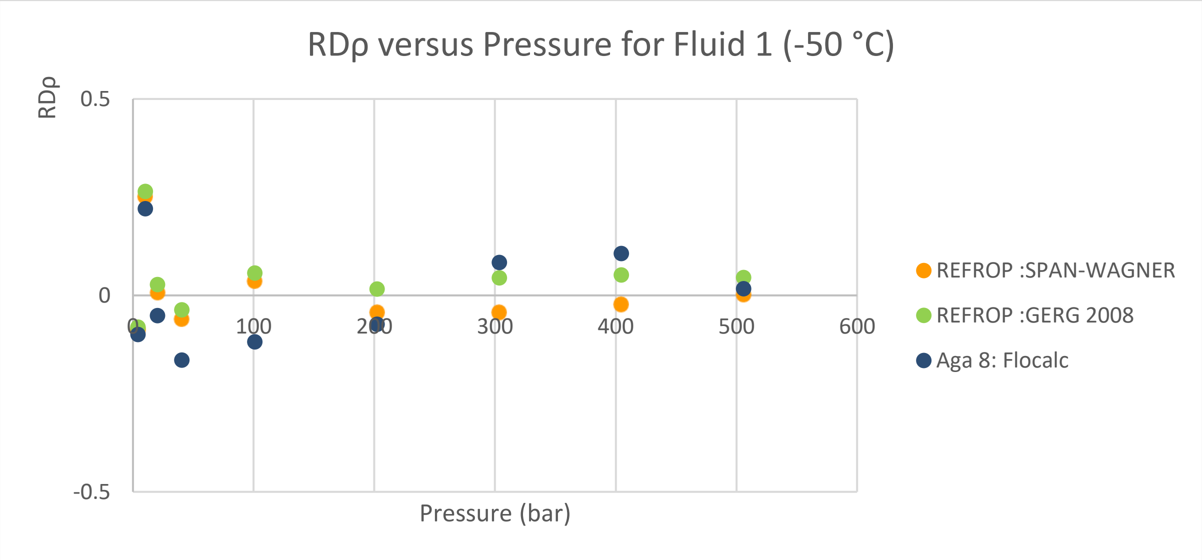

Figure 4 RDρ versus Pressure for Fluid 1 (-50 °C)

Data analysis at -50°C

- At –50 °C, the accuracy order is identical to the –75 °C case. Especially at pressures higher than 20 bar.
- Span–Wagner and GERG remain the best EOS, with almost negligible deviations.
- AGA 8 provides fairly good predictions, much better than cubic EOS.
- SRK is acceptable only for rough approximations.
- PR is unsuitable due to large and systematic overprediction.

Temperature 0 °C

Pressure (bar)	Span Wagner	GERG	PR	SRK	AGA 8
4.07	0.205	0.209	0.351	0.240	0.204
10.13	0.446	0.455	0.803	0.530	0.443
20.25	-0.287	-0.273	0.401	-0.129	-0.294
40.49	-0.125	-0.108	1.175	0.159	-0.137
80.90	0.015	0.026	2.346	0.480	0.001
121.21	0.023	0.027	3.171	0.594	0.015
202.32	0.043	0.052	4.355	0.668	0.065
404.56	0.018	0.048	5.520	0.185	-0.009
504.75	0.048	0.068	5.640	-0.191	-0.192
AADp	0.135	0.141	2.640	0.353	0.151

Table 6: Fluid 1 RDp and AADp for each EoS at 0°C

Since PR is clearly less accurate once compared against the experimental data, the chart below does not include PR to focus on the accuracy of the other EoS examined in this study.

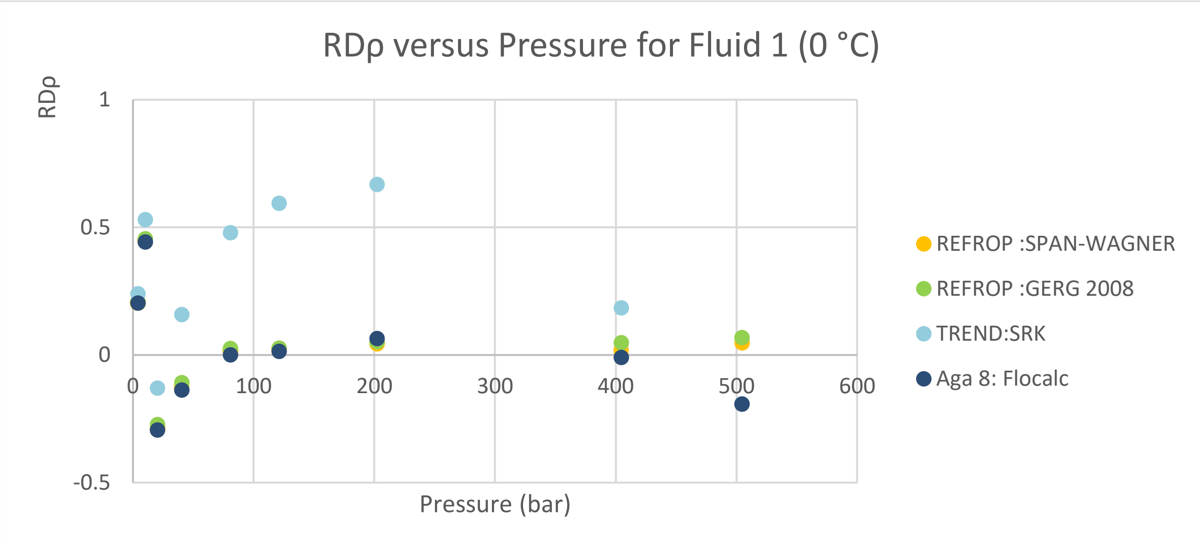

Figure 5: RDp versus Pressure for Fluid 1 (0 °C)

Data analysis at 0°C

- Span–Wagner and GERG are the most reliable EOS at 0 °C. Especially at pressures higher than 40 bar.
- PR is unsuitable in this condition due to overestimation as pressure increases.
- SRK performs moderately but still not precise.
- AGA 8 performs well and similar to Span-Wagner and GERG especially at pressures between 80 and 400 bar.

Temperature 25 °C

Pressure (bar)	Span Wagner	GERG	PR	SRK	AGA 8
1.22	0.85	0.85	0.89	0.86	0.85
1.51	0.56	0.56	0.61	0.57	0.56
5.09	0.41	0.41	0.57	0.44	0.41
10.42	0.00	0.01	0.32	0.07	0.00
19.77	-0.05	-0.04	0.54	0.07	-0.05
20.39	-0.10	-0.08	0.51	0.03	-0.09
31.09	0.07	0.08	0.97	0.25	0.07
40.56	-0.06	-0.05	1.08	0.17	-0.06
41.42	-0.07	-0.06	1.09	0.16	-0.07
53.11	-0.08	-0.06	1.37	0.21	-0.07
63.52	-0.04	-0.02	1.65	0.29	-0.03
82.56	0.00	0.00	2.09	0.38	0.01
102.80	-0.03	-0.02	2.45	0.40	-0.01
122.16	-0.03	-0.03	2.78	0.43	-0.02
122.99	-0.03	-0.03	2.80	0.44	-0.01
AADp	0.159	0.155	1.315	0.319	0.154

Table 7: Fluid 1 RDp and AADp for each EoS at 25°C

Since PR is clearly less accurate once compared against the experimental data, the chart below does not include PR to focus on the accuracy of the other EoS examined in this study.

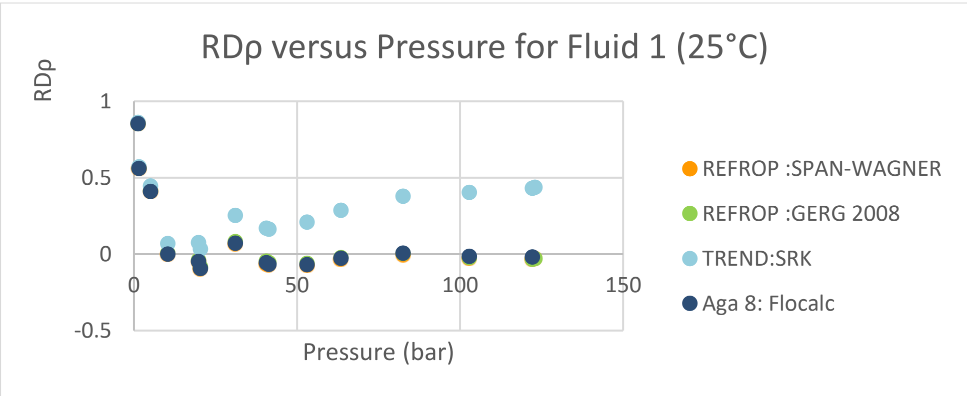

Figure 6: RDp versus Pressure for Fluid 1 (25 °C)

Data analysis at 25°C

- AGA 8 is the most reliable especially at pressures between 10 and 123 bar.
- Span–Wagner and GERG are equally as good and could be used.
- PR could only be used as an estimate at lower pressures but is unsuitable at pressures over 40 bar.
- SRK performs moderately could only be used accurately at pressures between 10 and 30 bar.

Temperature 50 °C

Pressure (bar)	Span Wagner	GERG	PR	SRK	AGA 8
1.190	0.933	0.934	0.966	0.940	0.934
1.340	0.664	0.665	0.702	0.672	0.665
5.120	0.275	0.279	0.415	0.304	0.277
10.300	-0.029	-0.022	0.248	0.027	-0.027
20.290	-0.050	-0.039	0.482	0.055	-0.045
29.740	-0.010	0.004	0.753	0.137	-0.003
45.270	-0.080	-0.066	1.035	0.125	-0.070
60.330	-0.051	-0.038	1.383	0.203	-0.039
81.190	-0.030	-0.021	1.808	0.278	-0.016
101.980	0.039	0.043	2.241	0.387	0.054
122.480	-0.080	-0.081	2.443	0.295	-0.065
122.500	-0.076	-0.077	2.447	0.299	-0.061
AADp	0.193	0.189	1.244	0.310	0.188

Table 8: Fluid 1 RDp and AADp for each EoS at 50°C

Since PR is clearly less accurate when compared to the experimental data, the chart below does not include PR to focus on the accuracy of the other EoS examined in this study.

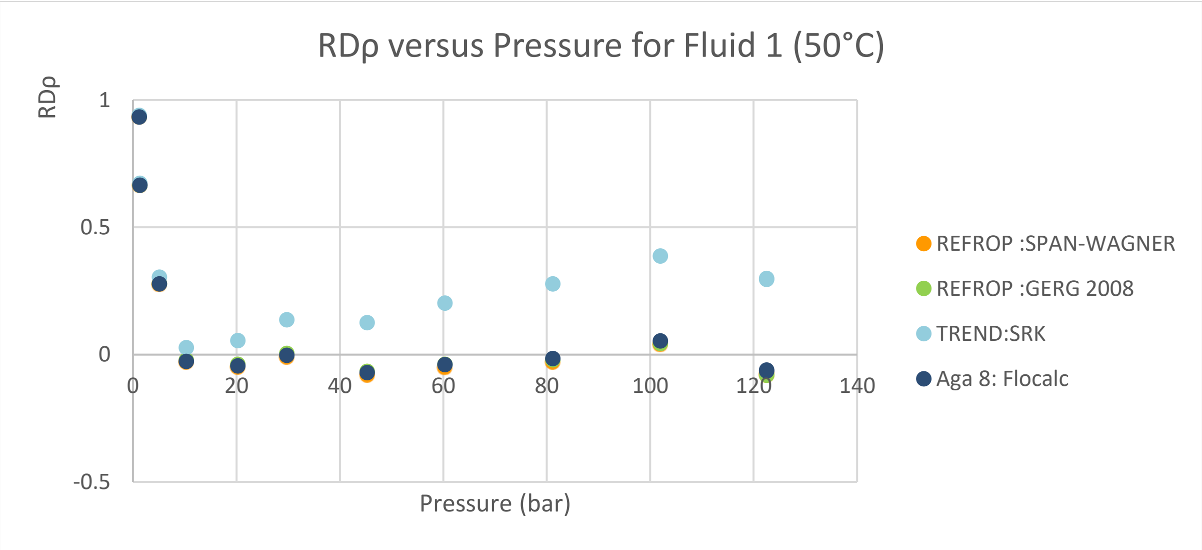

Figure 7: RDp versus Pressure for Fluid 1 (50 °C)

Focusing on pressures 10 bar and over and excluding the cubic equations. We will get the below visual representation.

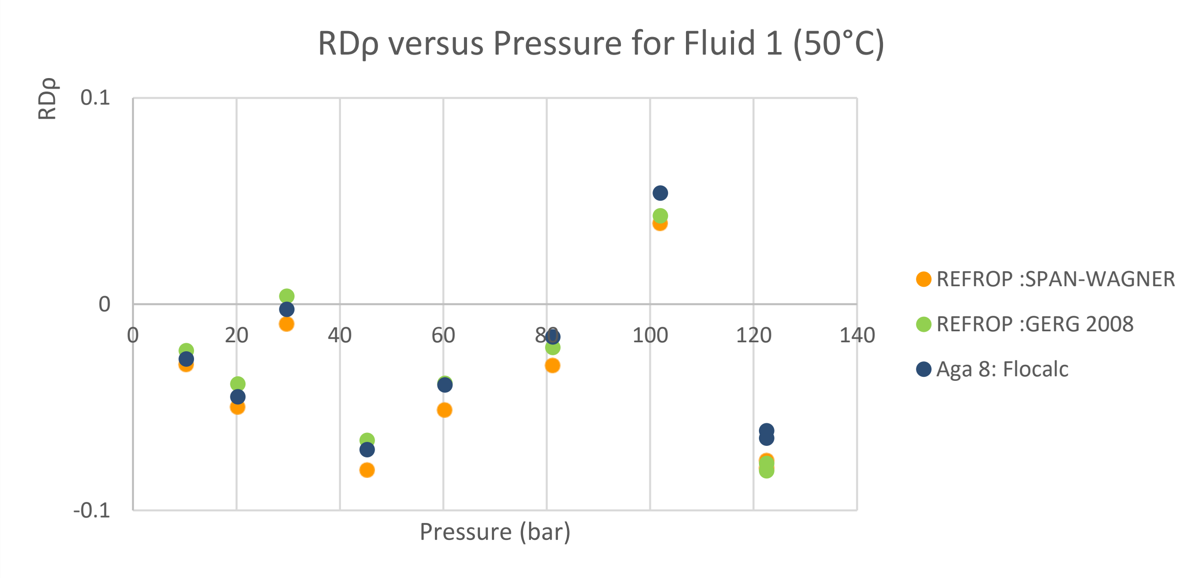

Figure 8: RDp versus Pressure for Fluid 1 (50 °C) excluding cubic equations

Data analysis at 50°C

- AGA 8 is the most reliable especially at pressures between 10 and 123 bar.
- Span–Wagner and GERG are equally as good and could be used.
- PR could only be used as an estimate at lower pressures but is unsuitable at pressures over 40 bar.
- SRK performs moderately could only be used accurately at pressures between 10 and 20 bar.

Temperature 75 °C

Pressure (bar)	Span Wagner	GERG	PR	SRK	AGA 8
1.190	0.878	0.878	0.907	0.883	0.878
1.260	0.792	0.793	0.823	0.798	0.792
5.070	0.323	0.326	0.446	0.346	0.323
5.090	0.431	0.435	0.555	0.455	0.432
10.130	0.042	0.048	0.284	0.087	0.043
20.240	-0.104	-0.093	0.367	-0.019	-0.103
31.250	0.034	0.047	0.744	0.158	0.036
45.720	-0.053	-0.040	0.950	0.114	-0.052
61.240	-0.026	-0.013	1.272	0.181	-0.025
82.750	-0.044	-0.035	1.627	0.205	-0.045
102.550	-0.053	-0.049	1.930	0.225	-0.055
122.200	-0.044	-0.045	2.221	0.253	-0.048
127.63	-0.046	-0.048	2.293	0.255	-0.051
AADp	0.221	0.219	1.109	0.306	0.222

Table 9: Fluid 1 RDp and AADp for each EoS at 75°C

Since PR is clearly less accurate when compared to the experimental data, the chart below does not include PR to focus on the accuracy of the other EoS examined in this study.

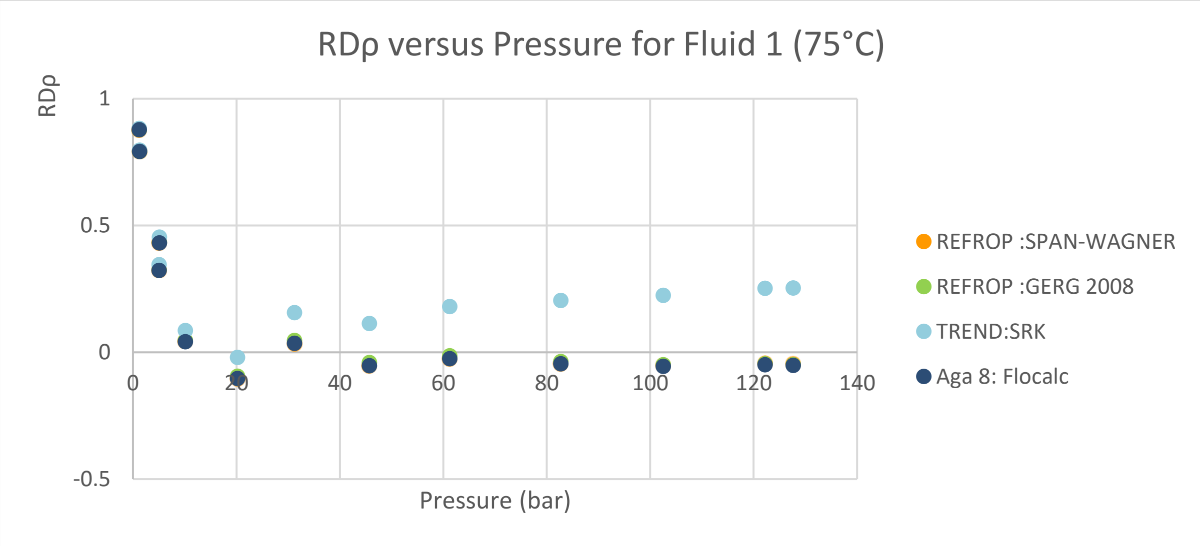

Figure 9: RDρ versus Pressure for Fluid 1 (75 °C)

Focusing on pressures 10 bar and over and excluding the cubic equations. We will get the below visual representation.

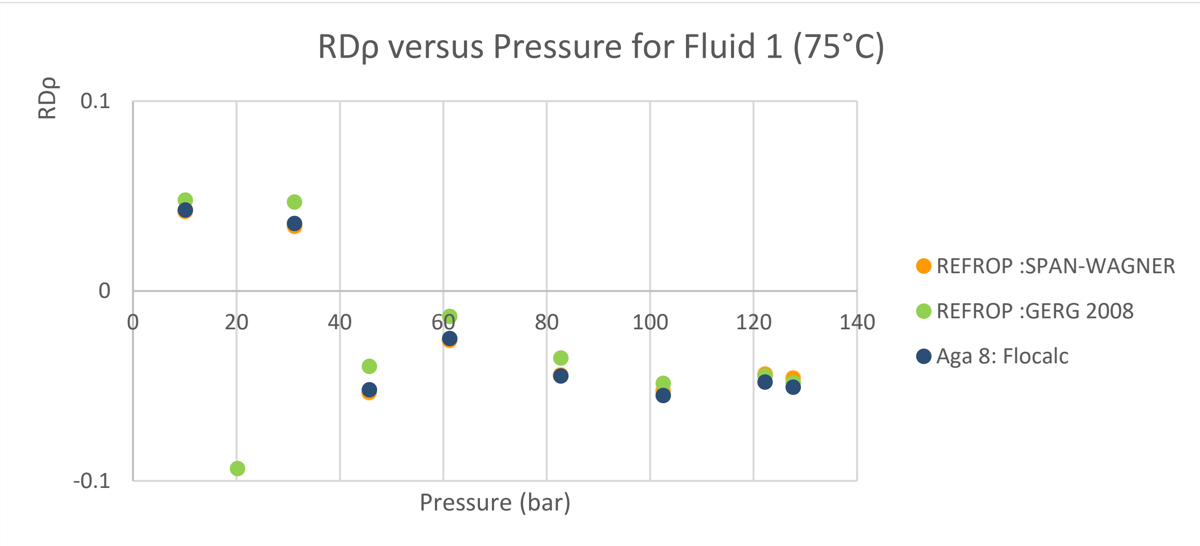

Figure 10: RDρ versus Pressure for Fluid 1 (75 °C) excluding cubic equations

Data analysis at 75°C

- Span–Wagner and GERG are the most reliable especially at pressures between 10 and 123 bar.
- AGA 8 is equally as good and could be used.
- PR could only be used as an estimate at lower pressures but is unsuitable at pressures over 40 bar.
- SRK performs moderately could only be used accurately at pressures between 10 and 20 bar.

Key Takeaways from F1 analysis

- Span–Wagner & GERG: Always the most accurate, valid across all temperatures and pressures.
- AGA 8: Strong performer, nearly matching Span–Wagner/GERG from 0–75 °C at all pressures; weaker at cryogenic/high temperatures.
- SRK: Moderate, only acceptable at 25–75 °C and low pressures (<100 bar).
- PR: Consistently worst EOS, with extreme overprediction at cryogenic/high P; only marginally usable at warm, low-pressure conditions.

EoS Pt Decision Map

	Temperature (°C)					
Pressure (bar)	-75	-50	0	25	50	75
4	AGA 8	GERG	AGA 8	Span-Wagner	Span-Wagner	Span-Wagner
10	Span-Wagner	AGA 8	AGA 8	Span-Wagner	GERG	Span-Wagner
20	AGA 8	Span-Wagner	SRK	GERG	GERG	SRK
30				Span-Wagner	AGA 8	Span-Wagner
40	GERG	GERG	GERG	GERG		
50				GERG	GERG	GERG
60				GERG	AGA 8	GERG
70						
80			AGA 8	GERG	AGA 8	GERG
100	Span-Wagner	Span-Wagner		AGA 8	Span-Wagner	GERG
120			AGA 8	AGA 8	AGA 8	Span-Wagner
200	GERG	GERG	Span-Wagner			
400	Span-Wagner	Span-Wagner	AGA 8			
500	Span-Wagner	Span-Wagner	Span-Wagner			

Table 10: EoS Pt decision map for fluid 1

Summary

In the 40–80 bar range, the advanced models (Span–Wagner, GERG, and AGA 8) all perform very similarly. At 0 °C, their deviations are within ±0.15 %. At 25 °C, the same three models remain tightly clustered, with deviations within ±0.1%, again showing almost indistinguishable performance. In contrast, PR shows much larger errors, already exceeding 1.0% by 40 bar and rising above 2.0% by 80 bar, while SRK is intermediate but still less accurate than the multiparameter models. Overall, Span–Wagner, GERG, and AGA 8 provide reliable and consistent predictions across 40–80 bar, while PR and SRK clearly underperform.

6.1.2 Fluid 2 (95% H_2 + 5% C_3H_8)

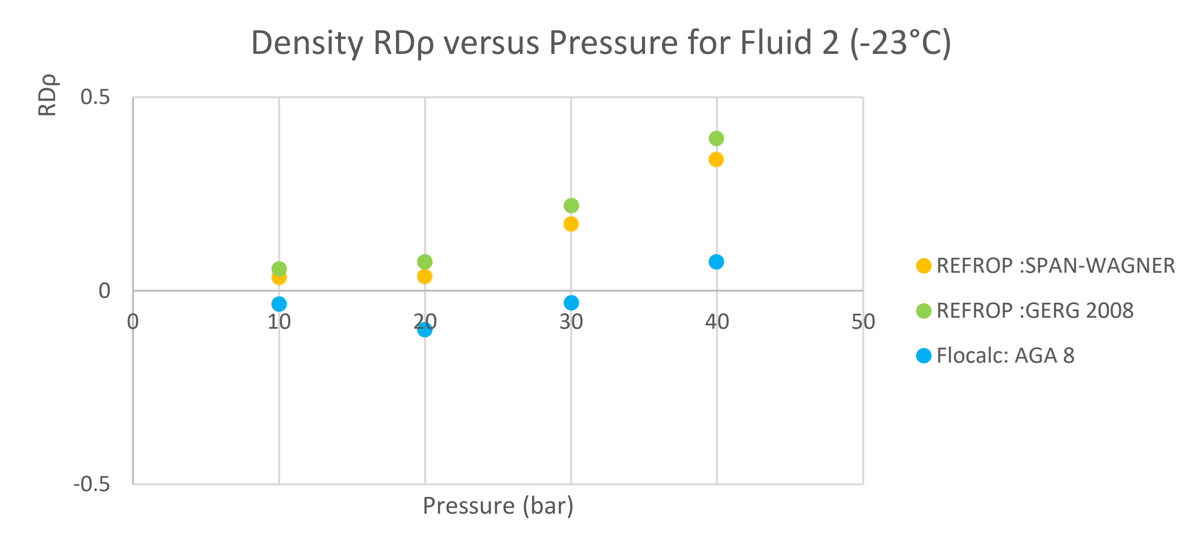

Figure 11: RDρ versus Pressure for Fluid 2 (-23 °C)

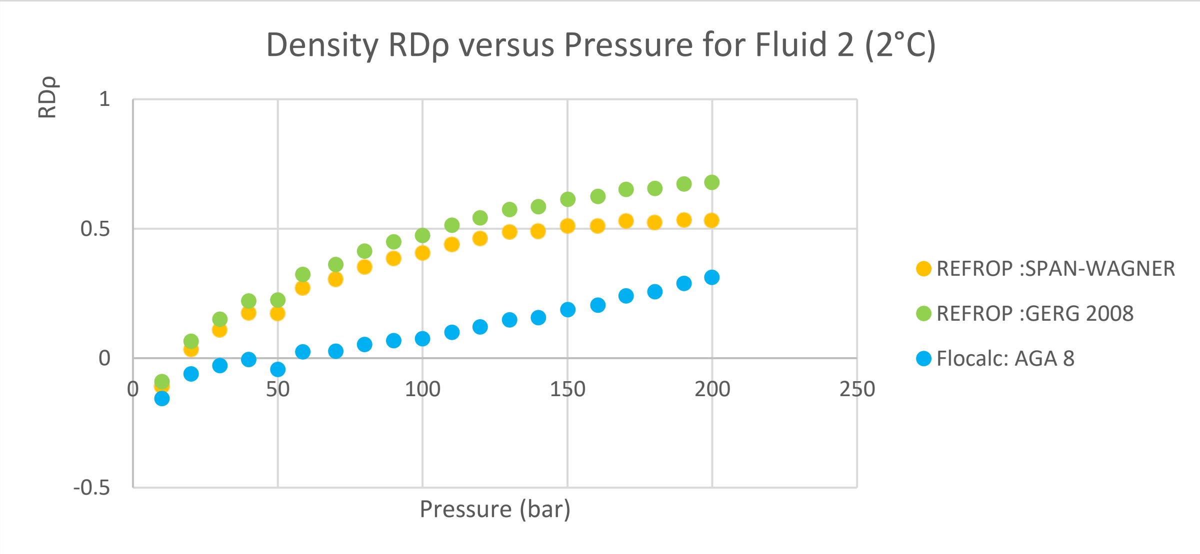

Figure 12: RDρ versus Pressure for Fluid 2 (2 °C)

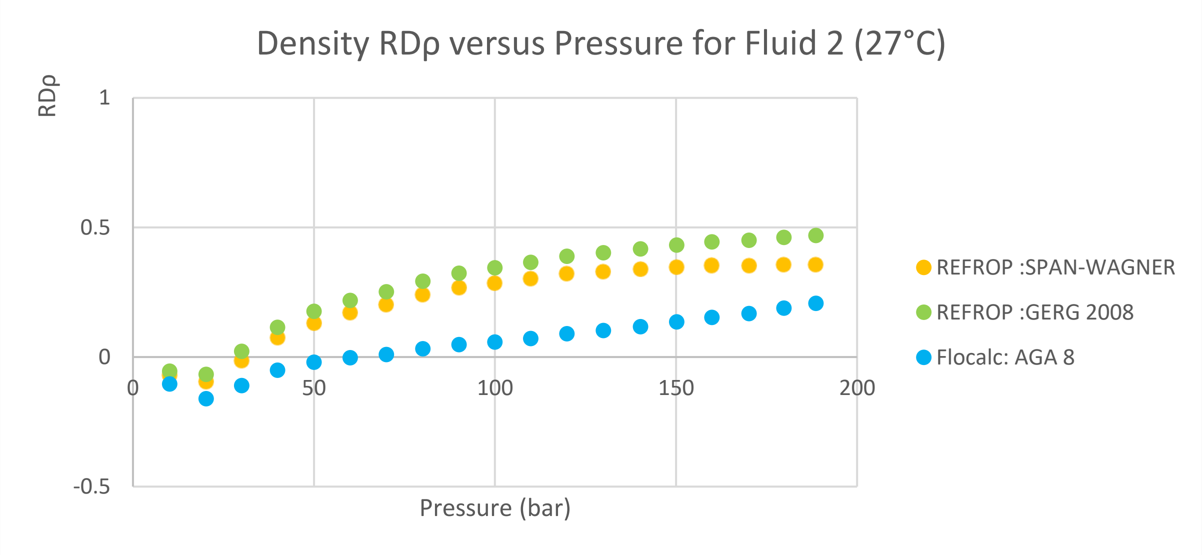

Figure 13: RDp versus Pressure for Fluid 2 (27 °C)

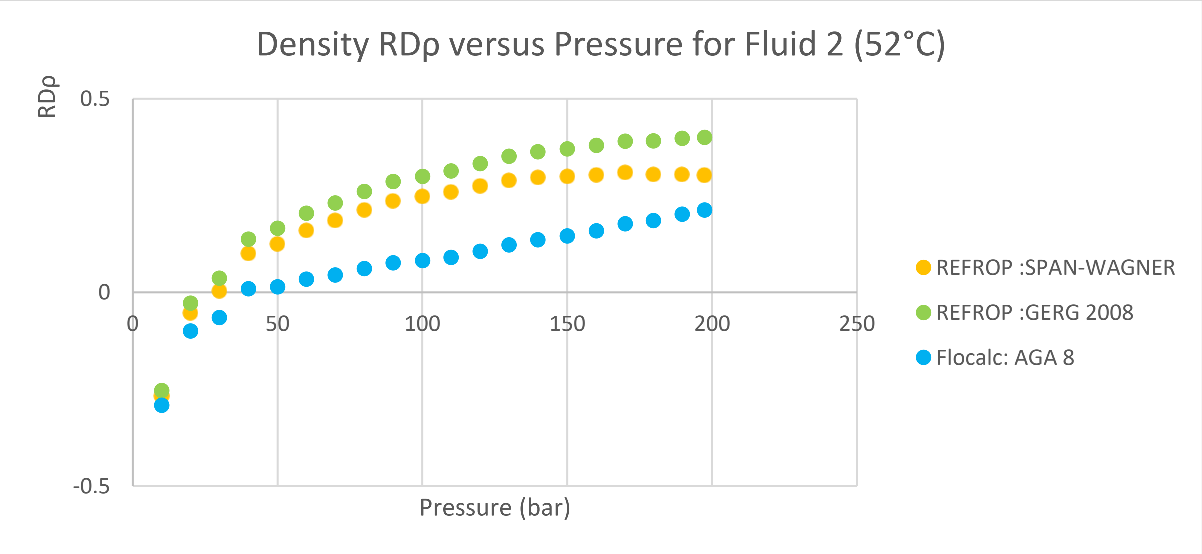

Figure 14: RDp versus Pressure for Fluid 2 (52 °C)

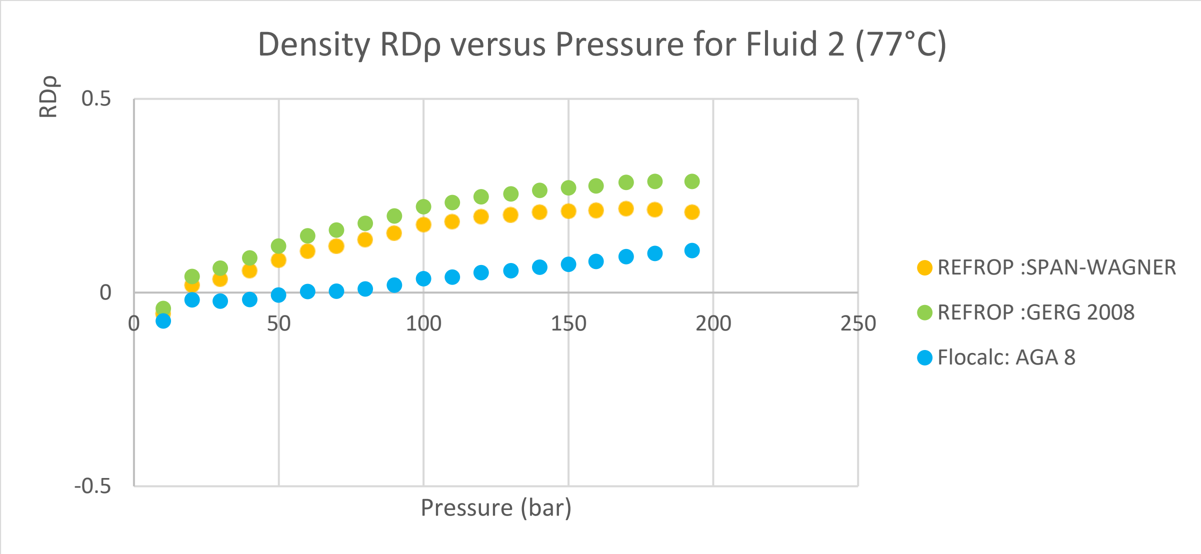

Figure 15: RDρ versus Pressure for Fluid 2 (77°C)

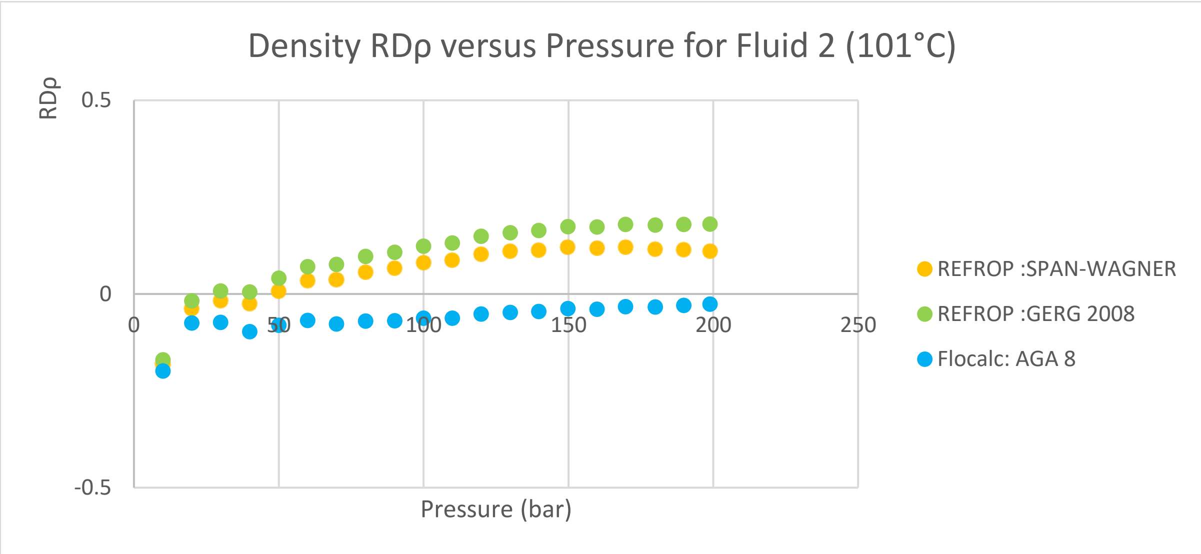

Figure 16: RDρ versus Pressure for Fluid 2 (101°C)

EoS	AADρ at (1- 40 bar)	AADρ at (10 - 200 bar)				
	-23 °C	2 °C	27 °C	52°C	77 °C	102°C
REFPROP	0.146	0.367	0.242	0.227	0.147	0.083
GERG	0.186	0.444	0.300	0.279	0.193	0.119
AGA 8	**0.060**	**0.128**	**0.096**	**0.116**	**0.046**	**0.064**

Table 11: Fluid 2 AADρ for each EoS

6.1.3 Fluid 3 (85% H_2 + 15% CH_4)

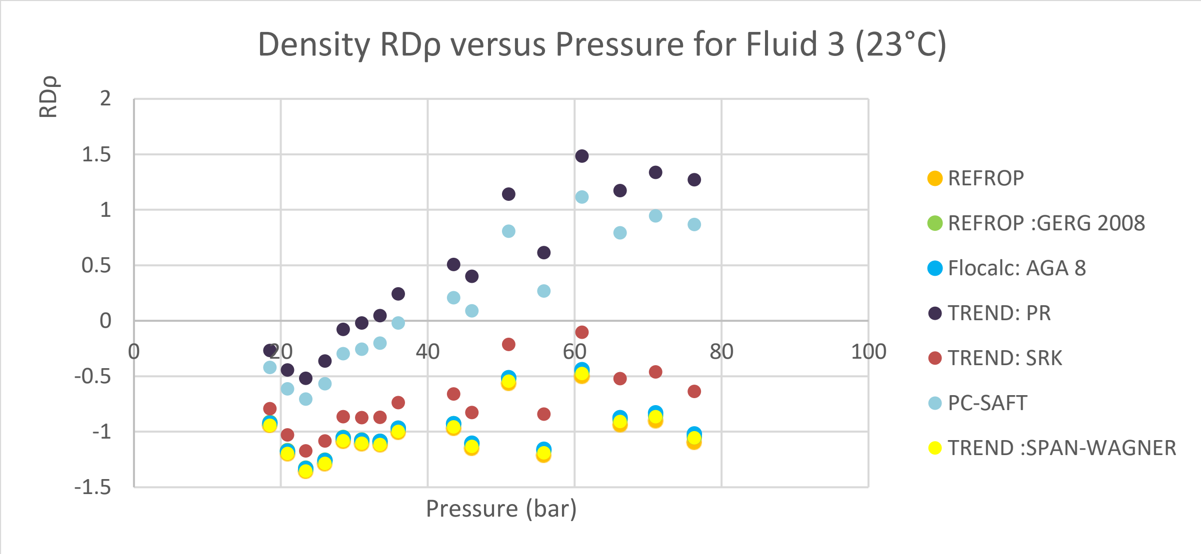

Figure 17: RDρ versus Pressure for Fluid 3 (23°C)

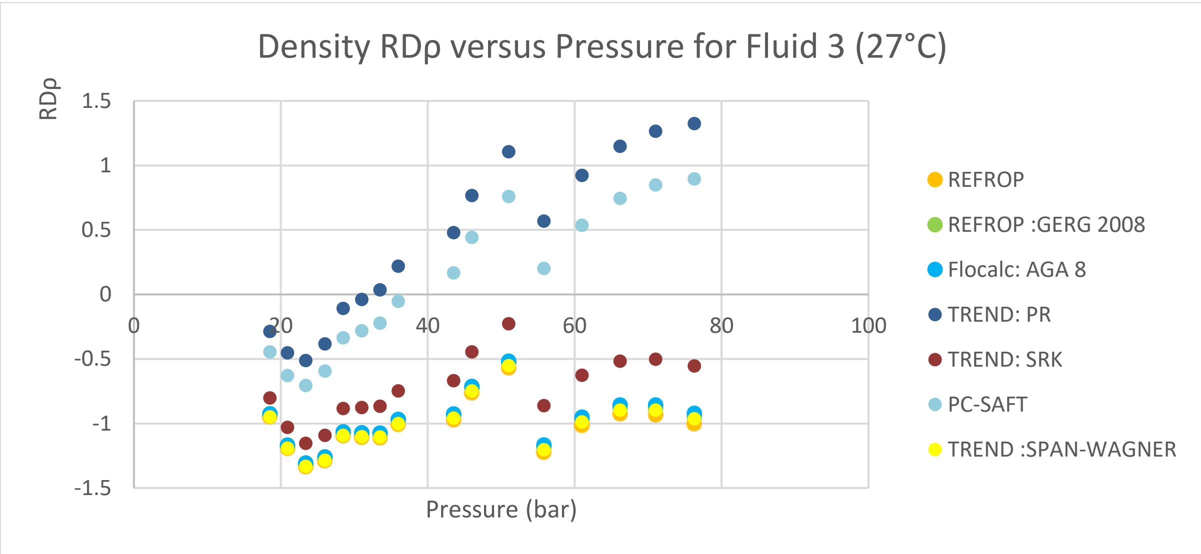

Figure 18: RDρ versus Pressure for Fluid 3 (27°C)

EoS	AADρ at (up to 76 bar)	
	23 °C	27 °C
REFPROP	1.026	1.031
GERG	0.987	0.992
Span - Wagner	1.011	1.017
AGA 8	0.983	0.985
PR	**0.427**	0.601
SRK	0.729	0.741
PC-SAFT	0.511	**0.491**

Table 12: Fluid 3 AADρ for each EoS

6.1.4 Fluid 4 (90% H_2 + 10% N_2)

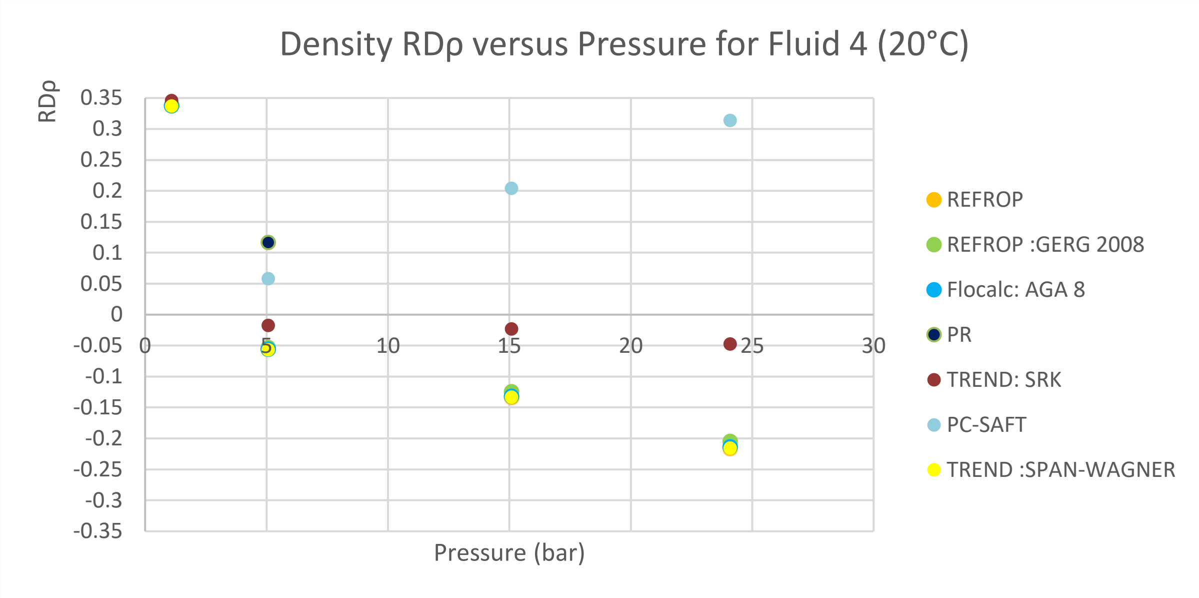

Figure 19: RDρ versus Pressure for Fluid 4 (20°C)

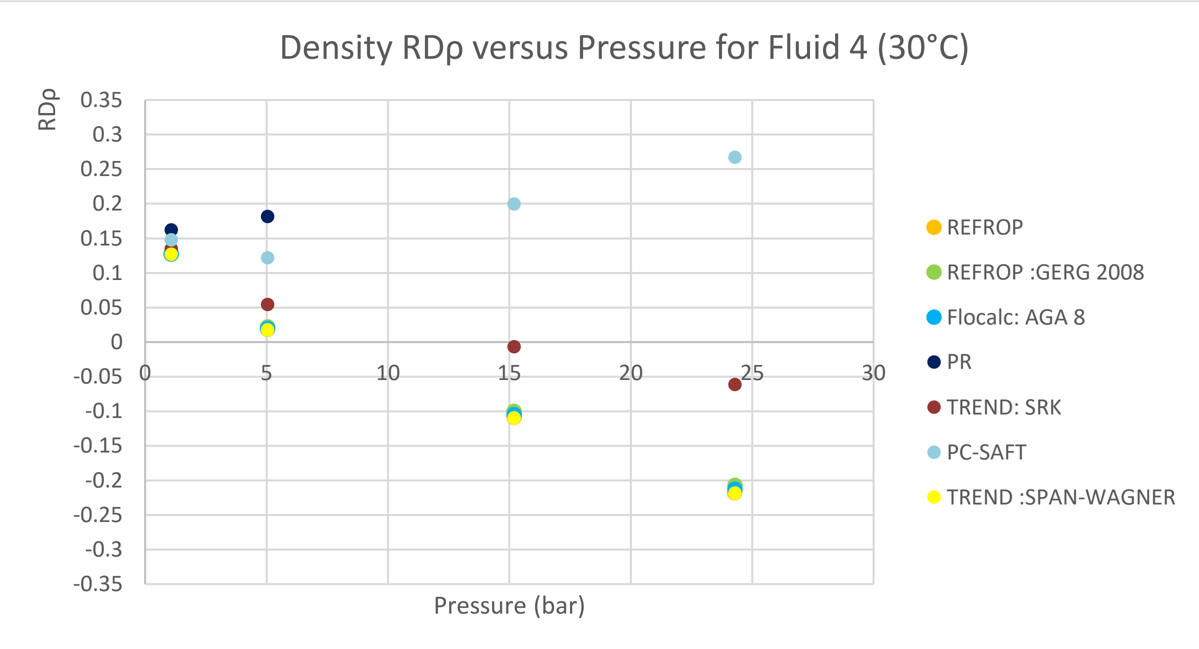

Figure 20: RDρ versus Pressure for Fluid 4 (30°C)

EoS	AADρ at (1 up to 24 bar)	
	20 °C	30 °C
REFPROP	0.186	0.118
GERG	0.180	0.114
Span - Wagner	0.186	0.118
AGA 8	0.185	0.116
PR	**0.071**	**0.041**
SRK	0.108	0.064
PC-SAFT	0.234	0.184

Table 13: Fluid 4 AADρ for each EoS

6.2 Viscosity

Fluid	H2	N2
1	0.9039	0.0961

Table 14: Composition used for hydrogen with impurities mixtures viscosity calculations

Note: Best EoS performance is highlighted in green.

6.2.1 Fluid 1 (90% H_2 + 10% N_2)

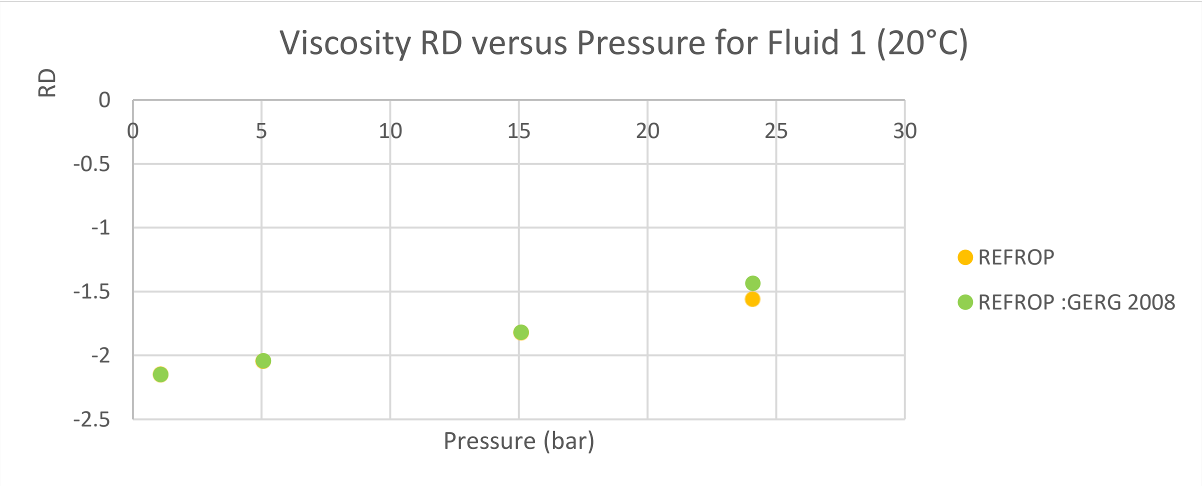

Figure 21: Viscosity RD versus Pressure for Fluid 1 (20°C)

.

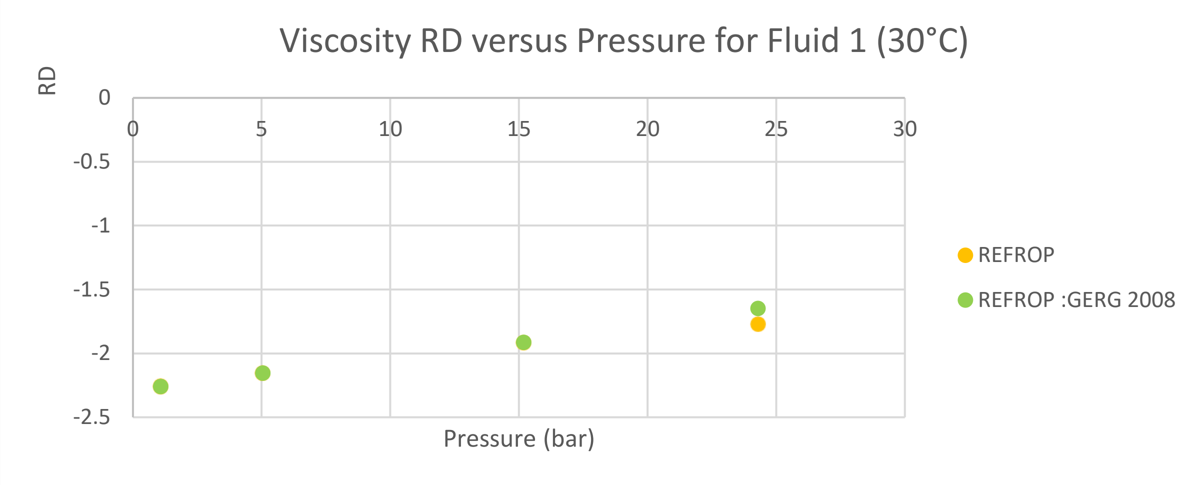

Figure 22: Viscosity RD versus Pressure for Fluid 1 (30°C)

EoS	AAD viscosity at (1 - 24 bar)	AAD viscosity at (1 - 24 bar)
	20 °C	30 °C
REFPROP	1.893	2.025
GERG	**1.861**	**1.993**

Table 15: Fluid 1 AAD viscosity for each EoS

6.3 Compressibility factor

Fluid	H2	C2H6
1	0.8	0.2

Table 16: Composition used for hydrogen with impurities mixtures viscosity calculations

Note: Best EoS performance is highlighted in green.

6.3.1 Fluid 1 (80% H_2 + 20% C_2H_6)

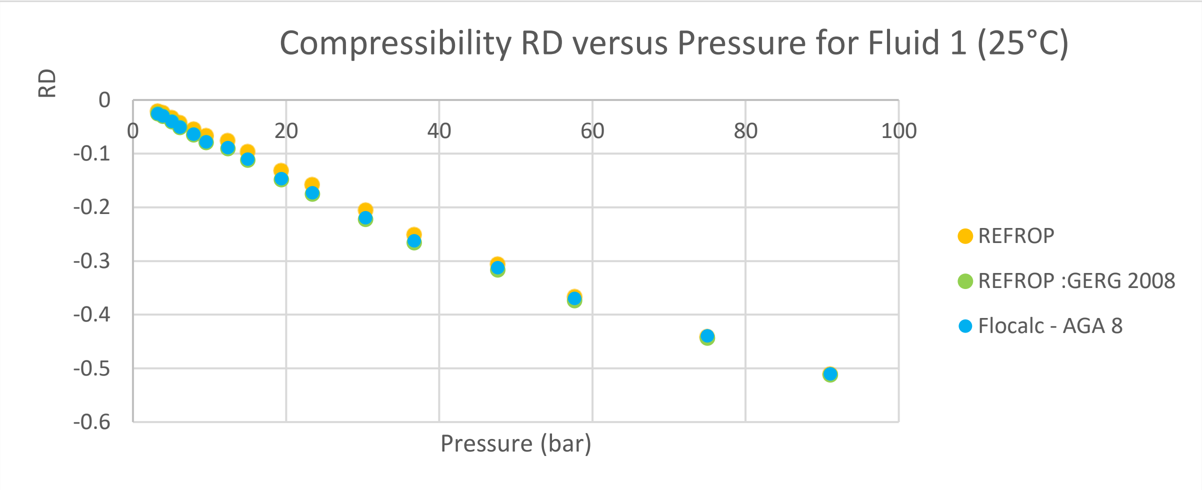

Figure 23: Compressibility RD versus Pressure for Fluid 1 (25°C)

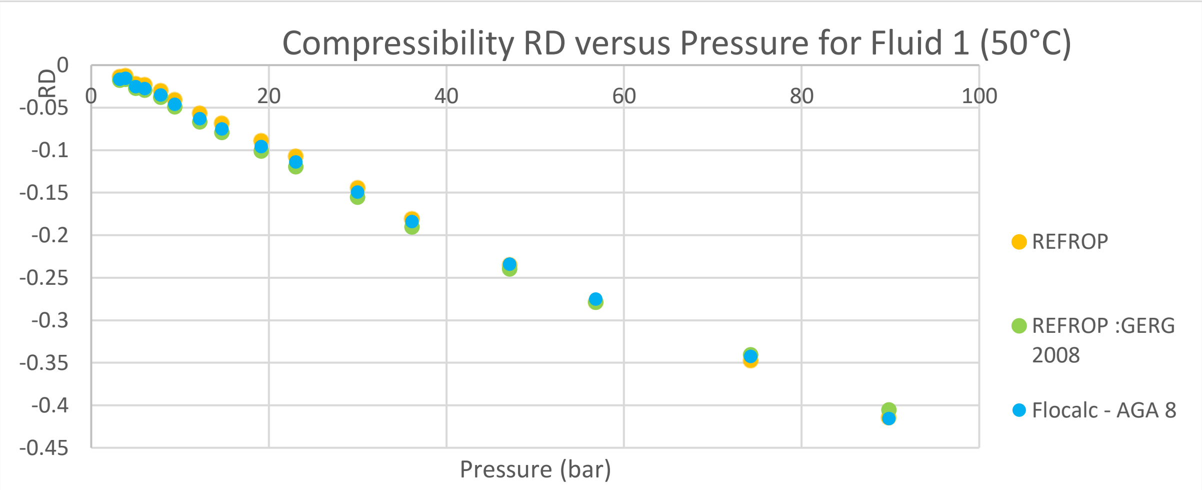

Figure 24: Compressibility RD versus Pressure for Fluid 1 (50°C)

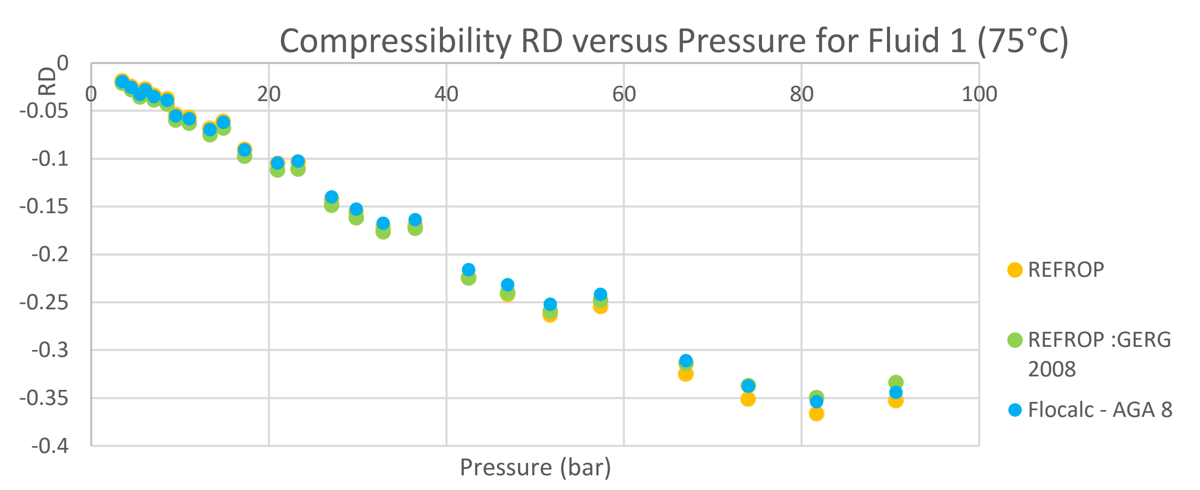

Figure 25: Compressibility RD versus Pressure for Fluid 1 (75°C)

EoS	AAD Z at (3-90 bar)		
	25 °C	50 °C	75 °C
REFPROP	**0.174**	**0.129**	0.149
GERG	0.184	0.135	0.150
AGA 8	0.182	0.132	**0.145**

Table 17: Fluid 1 AAD (Z) for each EoS

6.4 Discussion

This section discusses the analysis of each fluid, highlighting the main outcomes by examining the relationship between relative deviation (RD) and average absolute deviation (AAD) under defined process conditions. It also compares the performance of different EoS models and evaluates the influence of each mixture on density and other gas properties.

6.4.1 Density

For pure hydrogen and binary mixtures (>85% H_2, fluids 1–4), the pressure and temperature ranges included in the study are inconsistent and depend on the available experimental data. Based on the data, the pressure range covers 120 bar for pure hydrogen (fluid 1), up to 200 bar for the hydrogen–propane mixture (fluid 2), up to 76 bar for the hydrogen–methane mixture (fluid 3), and up to 24 bar for the hydrogen–nitrogen mixture (fluid 4). A wide range of temperatures is covered for fluids 1 and 2; however, for fluids 3 and 4, data are only available at around 20 °C and 30 °C. In some charts, EoS models with high RDρ values were omitted for simplicity but are still included in the corresponding tables.

It is worth noting that, the below statements are generic data analysis of the trend of RDρ density vs. pressure at different temperatures:

For pure hydrogen (fluid 1), the trends show that all three EoS models (GERG, Span–Wagner, and AGA 8) are suitable across the examined temperature and pressure ranges. Span–Wagner provides the lowest errors at temperatures below 0 °C, while AGA 8 performs best between 0 °C and 50 °C. The highest error (AADρ = 0.22%) is observed at 75 °C.

For the hydrogen–propane mixture with 95% H_2 (fluid 2), errors remain within ±0.13% for pressures of up to 200 bar and across temperatures from 2 °C to 102 °C. AGA 8 clearly outperforms GERG and REFPROP, demonstrating its ability to handle hydrogen–propane mixtures at high hydrogen concentrations (>95% H_2) especially at lower temperatures. At -23 °C, the experimental data are limited, with pressures only extending to 40 bar.

For the hydrogen–methane and hydrogen–nitrogen mixtures, the limited availability of experimental data affects the reliability of the calculated AADρ values. For the hydrogen–nitrogen binary mixture, the PR model gives the lowest errors under the examined conditions, although the datasets extend only up to 24 bar. For the hydrogen–methane binary mixture at 85% H_2, PR performs best at 23 °C, but its error increases significantly at slightly higher temperatures. At 27 °C, the PC-SAFT model provides the best performance. However, the limited experimental data (restricted to pressures up to 76 bar and temperatures of only 23 °C and 27 °C) highlights the weaknesses of the dataset for hydrogen–methane mixtures.

6.4.2 Other Gas Properties (Viscosity & Compressibility factor)

Limited data were available for examining both viscosity and compressibility factors. The effect of high hydrogen content on viscosity was analysed using a hydrogen–nitrogen mixture with 90% H_2, although the available pressure data only extended only up to 24 bar. The effect of high hydrogen concentration on the compressibility factor was evaluated using a hydrogen–ethane mixture with 80% H_2.

It is worth noting that, the below statements are generic data analysis of the trend of RD Viscosity and RD Z vs. pressure at different temperatures:

For the hydrogen–nitrogen mixture, viscosity errors are high for both REFPROP and GERG. The relative deviation (RD) decreases as pressure and temperature increase. At lower pressures, REFPROP and GERG perform similarly, but at the highest available pressure (24 bar), GERG clearly performs better.

For the hydrogen–ethane mixture, the compressibility factor results show that REFPROP, GERG, and AGA 8 perform very similarly under the examined process conditions, with RD increasing as pressure rises up to 80 bar. REFPROP is slightly more accurate at 25 °C and 50 °C, whereas AGA 8 performs best at 75 °C.

7 Natural gas with up to 20% Hydrogen (H_2)

7.1 Density

Composition

Fluid	H2	CH4	C2H6	C3H8	iC4	nC4	iC5	nC5	neoC5	C6	N2	Co2	He
1	0.03	0.7885	0.0075	0.003	0.002	0.002	0.0005	0.0005	0.0005	0.0005	0.12	0.04	0.005
2	0.05	0.836	0.057	0.019	0.0019	0.00285					0.01425	0.019	
3	0.1	0.792	0.054	0.018	0.0018	0.0027					0.0135	0.018	
4	0.15	0.748	0.051	0.017	0.0017	0.00255					0.01275	0.017	
5	0.20	0.704	0.048	0.016	0.0016	0.0024					0.012	0.016	
6	0.05	0.95											
7	0.0858	0.9142											
8	0.1	0.9											
9a	0.2005	0.7995											
9b	0.2031	0.7969											

Table 18: Composition used for NG with up to 20% hydrogen mixtures density calculations

Additional Composition

Fluid	H2	CH4	C2H6	C3H8	iC4	nC4	iC5	nC5	C6	N2	Co2
1a	0.0278	0.9072	0.0255	0.00408	0.000583	0.000585	0.000192	0.000195	0.000587	0.0238	0.00952
3a	0.0999	0.8467	0.024	0.00383	0.000479	0.000484	0.000197	0.000199	0.000607	0.0149	0.00867
4a	0.155	0.7947	0.0225	0.00361	0.000537	0.000672	0.000192	0.000194	0.000316	0.0138	0.00852
5a	0.201	0.7512	0.0216	0.00334	0.000537	0.000819	0.000192	0.000195	0.000381	0.0129	0.00786

Table 19: Additional Composition used for NG with up to 20% hydrogen mixtures density calculations

Note: Additional analysis was performed on the mixtures listed below to investigate the effect of H_2 blending with natural gas. The experimental data were obtained from the study "Density Characterization of Hydrogen–Blended Natural Gas Using a Single-Sinker Densimeter" [8]*, an external source outside the HYCCS database.*

Note: Best EoS performance is highlighted in green.

7.1.1 Fluid 1 (3% H_2 + NG)

Temperature -13.1 °C

Pressure (bar)	REFPROP	GERG	AGA 8
9.99	-0.022	-0.023	-0.002
19.98	-0.017	-0.022	0.013
29.93	0.004	0.000	0.040
40.01	0.029	0.024	0.068
49.99	0.018	0.012	0.052
60.01	0.041	0.035	0.063
70.07	0.058	0.048	0.058
80.10	0.093	0.081	0.063
90.05	0.125	0.111	0.060
100.08	0.168	0.150	0.060
110.09	0.214	0.190	0.060
120.11	0.261	0.232	0.072
130.12	0.304	0.271	0.083
140.11	0.335	0.299	0.094
150.12	0.359	0.314	0.108
160.10	0.365	0.322	0.124
170.08	0.362	0.317	0.140
180.10	0.354	0.311	0.163
190.11	0.346	0.300	0.185
198.43	0.334	0.285	0.200
AADρ	0.190	0.167	0.085

Table 20 Fluid 1 RDρ and AADρ for each EoS at -13°C

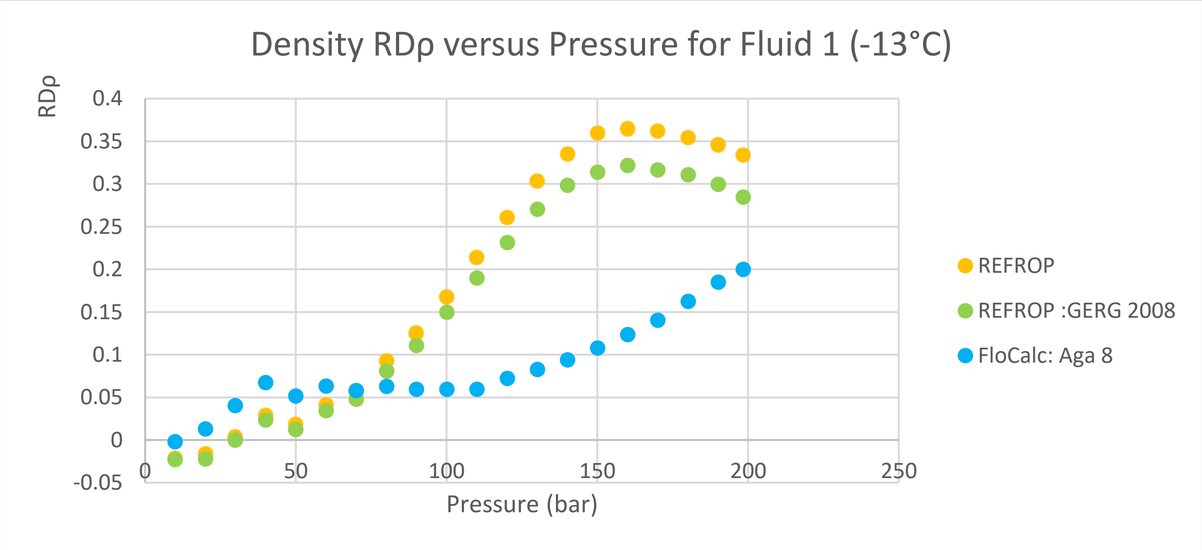

Figure 26: RDρ versus Pressure for Fluid 1 (-13 °C)

Data analysis at -13°C for F1

- REFPROP: widely used, but here it overpredicts slightly at mid-range and shows more scatter.
- GERG: similar to REFPROP, slightly better at lower pressures.
- AGA 8: most accurate and consistent across full pressure range especially over 80 bar.

Temperature 1.8 °C

Pressure (bar)	REFPROP	GERG	AGA 8
9.99	-0.017	-0.018	-0.004
20.00	0.024	0.024	0.043
30.01	-0.008	-0.012	0.016
40.06	0.028	0.025	0.051
50.03	0.033	0.029	0.052
60.00	0.060	0.054	0.071
70.01	0.076	0.067	0.072
80.02	0.089	0.077	0.066
90.03	0.106	0.093	0.062
100.06	0.141	0.126	0.072
110.04	0.153	0.135	0.060
120.06	0.196	0.171	0.076
130.07	0.213	0.191	0.076
140.08	0.235	0.214	0.081
150.04	0.260	0.234	0.094
160.06	0.272	0.242	0.098
170.13	0.288	0.254	0.110
180.08	0.292	0.254	0.119
92.34	0.286	0.250	0.131
AADρ	0.146	0.130	0.071

Table 21 Fluid 1 RDρ and AADρ for each EoS at 1.8°C

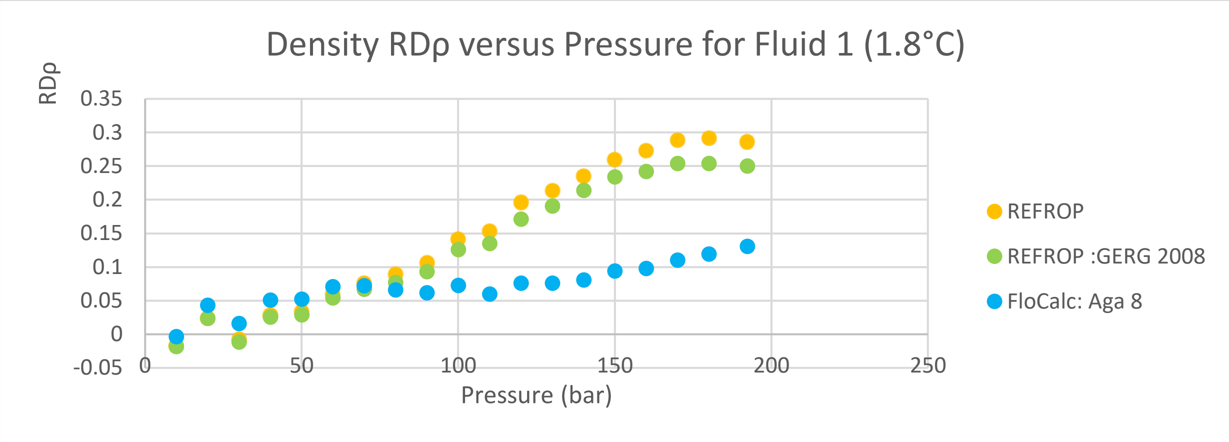

Figure 27: RDρ versus Pressure for Fluid 1 (1.8 °C)

Data analysis at 1.8°C for F1

- REFPROP: Tends to overpredict at higher pressures.
- GERG: Slightly better than REFPROP but follows the same trend.
- AGA 8: The most accurate and pressure-stable - Significantly lower AADρ, better suited for scenarios more than 80 bar.

Temperature 26.8 °C

Pressure (bar)	REFPROP	GERG	AGA 8
9.99	0.045	0.044	0.051
19.99	-0.007	-0.007	0.005
29.91	0.013	0.013	0.025
39.98	0.006	0.006	0.017
49.99	0.035	0.035	0.042
59.99	0.051	0.047	0.052
70.02	0.061	0.056	0.053
80.00	0.069	0.062	0.053
90.01	0.082	0.071	0.053
100.02	0.101	0.089	0.061
110.00	0.111	0.097	0.058
120.03	0.129	0.120	0.067
130.03	0.145	0.128	0.071
140.02	0.161	0.136	0.072
150.02	0.172	0.149	0.077
160.03	0.186	0.165	0.082
170.02	0.193	0.166	0.082
180.03	0.202	0.177	0.086
190.09	0.207	0.182	0.090
198.51	0.207	0.178	0.090
AADρ	0.109	0.096	0.059

Table 22 Fluid 1 RDρ and AADρ for each EoS at 26.8°C

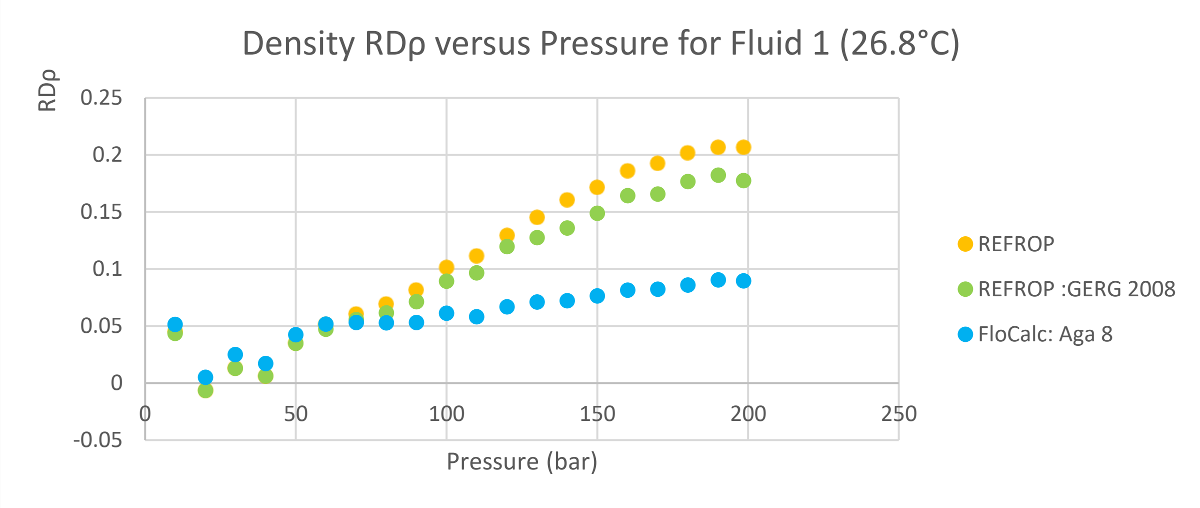

Figure 28: RDp versus Pressure for Fluid 1 (26.8 °C)

Data analysis at 26.8°C for F1

- REFPROP & GERG: Reasonable at low pressures, but accuracy deteriorates with pressure.
- AGA 8: Performs best overall, especially at higher pressures (>70 bar), making it the most reliable choice.

Temperature 51.8 °C

Pressure (bar)	REFPROP	GERG	AGA 8
9.98	-0.039	-0.040	-0.035
19.99	0.021	0.014	0.024
29.85	-0.014	-0.014	-0.009
39.98	-0.003	-0.003	0.002
49.99	0.022	0.022	0.025
59.98	0.018	0.018	0.016
69.99	0.025	0.023	0.019
79.99	0.040	0.037	0.027
89.99	0.048	0.042	0.029
99.99	0.061	0.053	0.034
110.00	0.077	0.066	0.044
120.01	0.093	0.080	0.052
130.02	0.102	0.087	0.055
140.01	0.106	0.087	0.056
149.98	0.112	0.094	0.056
160.00	0.125	0.101	0.060
170.00	0.138	0.115	0.065
179.99	0.136	0.114	0.062
190.01	0.144	0.116	0.064
199.28	0.145	0.119	0.063
AADp	0.074	0.062	0.040

Table 23 Fluid 1 RDp and AADp for each EoS at 51.8°C

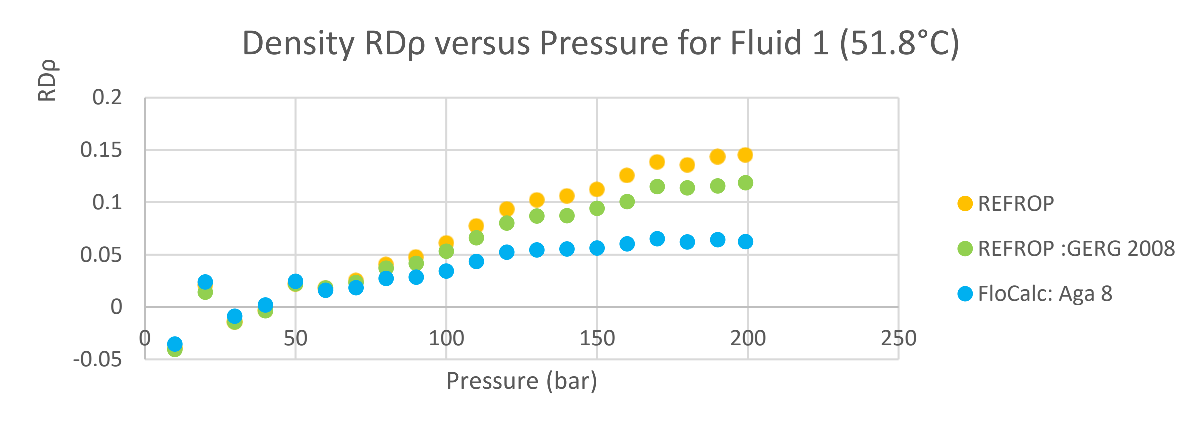

Figure 29: RDp versus Pressure for Fluid 1 (51.8 °C)

Data analysis at 51.8°C for F1

- AGA 8 performs the best in both accuracy and stability.
- GERG provides a moderate improvement over REFPROP.
- REFPROP shows the largest deviations, especially at higher pressures but is still within acceptable range.

Temperature 76.8 °C

Pressure (bar)	REFPROP	GERG	AGA 8
9.99	0.034	0.033	0.037
19.99	0.031	0.031	0.035
29.85	0.036	0.036	0.039
39.98	0.030	0.030	0.034
49.98	0.027	0.027	0.028
59.98	0.048	0.048	0.046
69.97	0.038	0.038	0.034
79.98	0.048	0.048	0.041
89.98	0.059	0.058	0.047
99.97	0.068	0.065	0.051
109.96	0.076	0.071	0.054
119.91	0.085	0.076	0.058
129.98	0.104	0.094	0.073
139.98	0.109	0.095	0.074
149.96	0.117	0.108	0.079
159.98	0.125	0.106	0.085
169.95	0.130	0.112	0.085
179.97	0.140	0.115	0.087
190.00	0.138	0.122	0.090
199.41	0.148	0.126	0.090
AADp	0.080	0.072	0.058

Table 24 Fluid 1 RDp and AADp for each EoS at 76.8°C

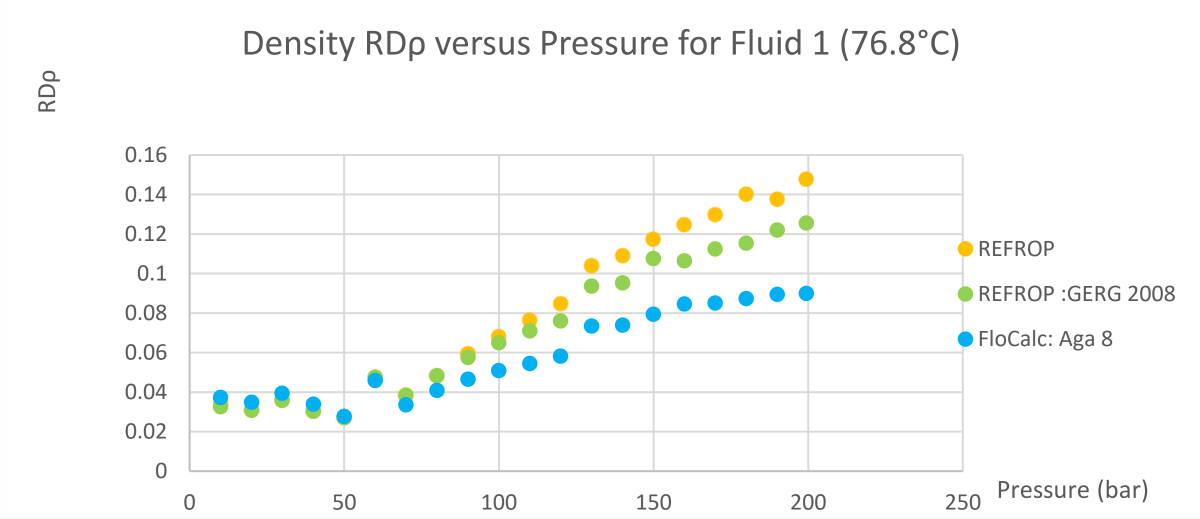

Figure 30: RDρ versus Pressure for Fluid 1 (76.8 °C)

Data analysis at 76.8°C for F1

- AGA 8 continues to provide the best balance of accuracy and stability.
- GERG is moderately better than REFPROP but still shows larger deviations at high pressures.
- All three models perform similarly at low pressures (<50 bar), but differences grow with pressure (>100 bar).

Key Takeaways from F1 analysis

- AGA 8 consistently has the lowest AADρ and highest accuracy across all temperatures.
- GERG is slightly better than REFPROP, but both show larger deviations than AGA 8.
- REFPROP has the highest deviations, especially at lower temperatures and higher pressures.

EoS Pt Decision Map

	Temperature (°C)				
Pressure (bar)	-13.1	1.8	26.8	51.8	76.8
10	AGA 8	AGA 8	GERG	AGA 8	GERG
20	AGA 8	REFPROP	AGA 8	GERG	REFPROP
30	GERG	REFPROP	REFPROP	AGA 8	REFPROP
40	GERG	GERG	REFPROP	AGA 8	REFPROP
50	GERG	GERG	REFPROP	REFPROP	REFPROP
60	GERG	GERG	GERG	AGA 8	AGA 8
70	GERG	GERG	AGA 8	AGA 8	AGA 8
80	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
90	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
100	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
110	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
120	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
130	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
140	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
150	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
160	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
170	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
180	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
190	AGA 8	AGA 8	AGA 8	AGA 8	AGA 8
200	AGA 8		AGA 8	AGA 8	AGA 8

Table 25: EoS Pt decision map for fluid 1

Summary

Between 40 and 80 bar, the three equations of state (REFPROP, GERG, and AGA 8) show broadly similar performance at both 1.8 °C and 26.8 °C, with only modest differences in deviations (RDρ<0.1%). The absolute differences in deviations are small across this entire region, meaning that any of the models would provide reasonably consistent predictions without large discrepancies.

7.1.2 Fluid 1a (3% H_2 + NG)

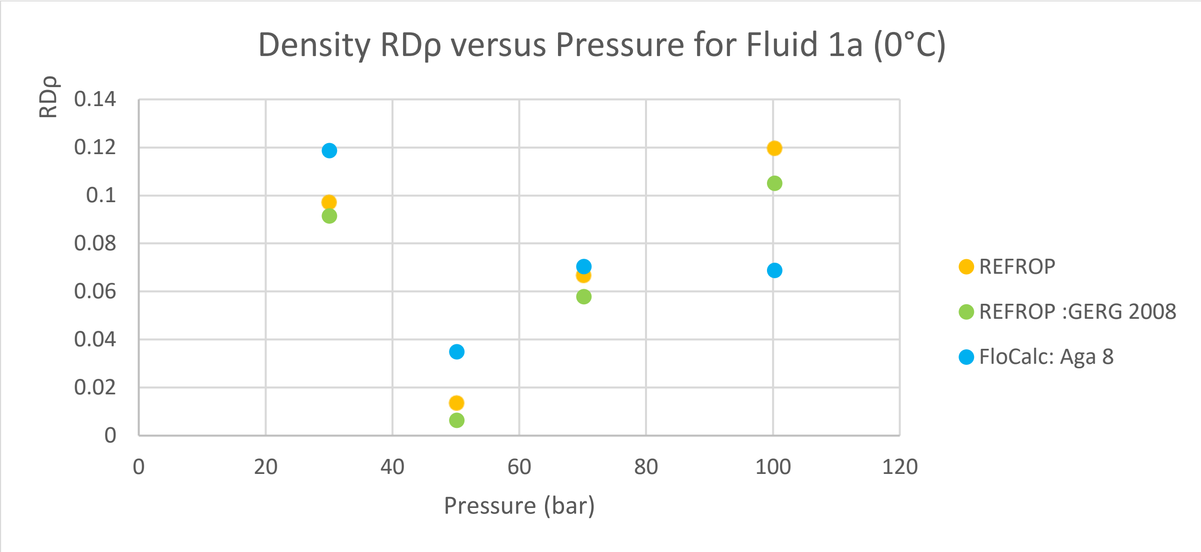

Figure 31: RDρ versus Pressure for Fluid 1a (0 °C)

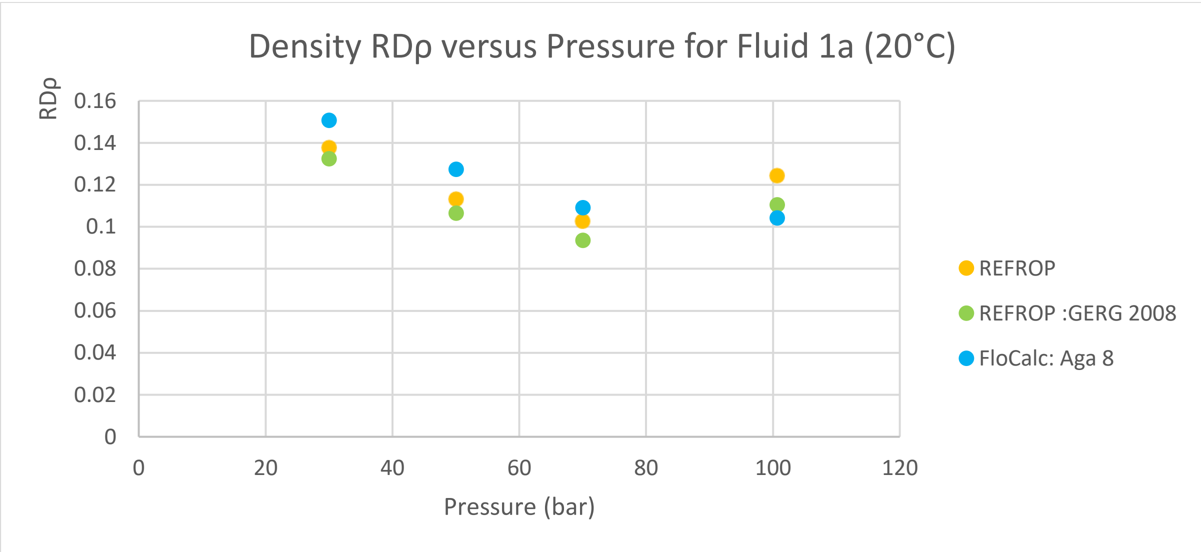

Figure 32: RDρ versus Pressure for Fluid 1a (20 °C) 2

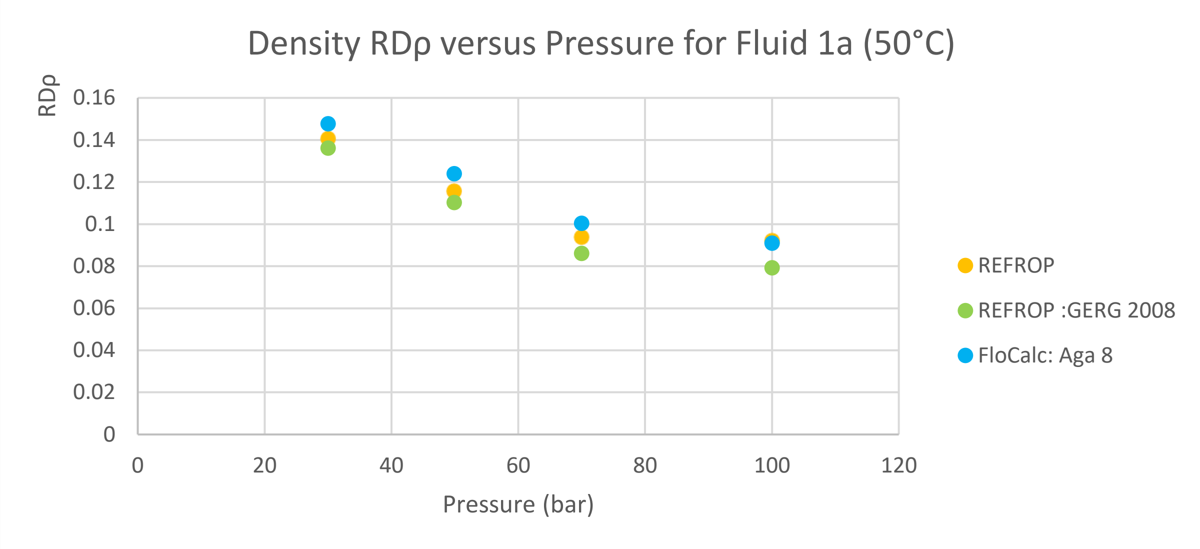

Figure 33: RDρ versus Pressure for Fluid 1a (50 °C) 3

EoS	AADρ at (30 up to 100 bar)		
	0 °C	20°C	50 °C
REFPROP	0.074	0.119	0.111
GERG	**0.065**	**0.111**	**0.103**
AGA 8	0.073	0.123	0.116

Table 26: Fluid 1a AADρ for each EoS

7.1.3 Fluid 2 (5% H_2 + NG)

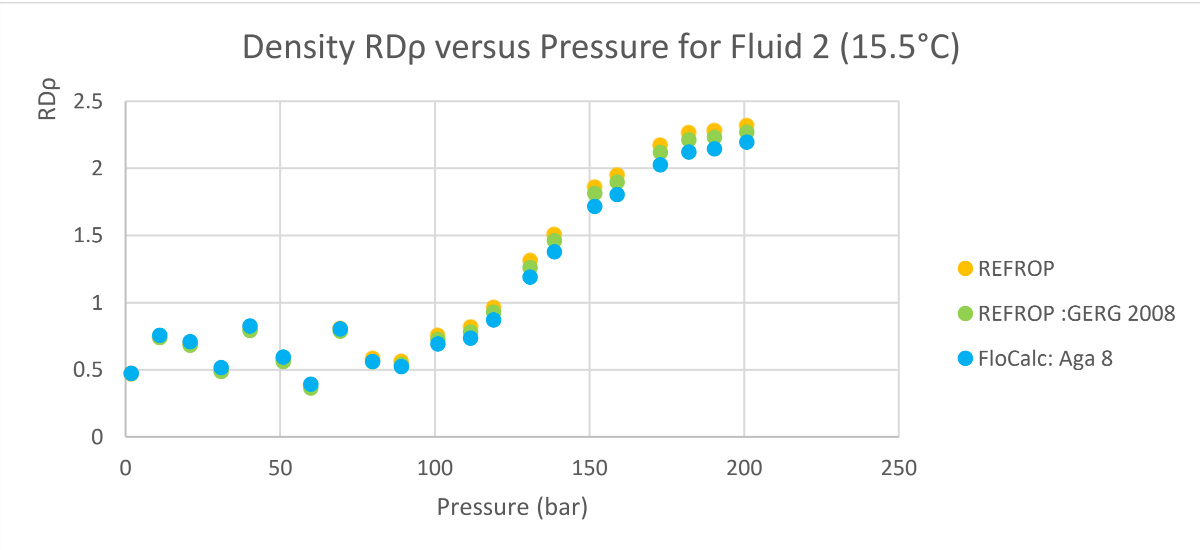

Figure 34: RDρ versus Pressure for Fluid 2 (15.5 °C)

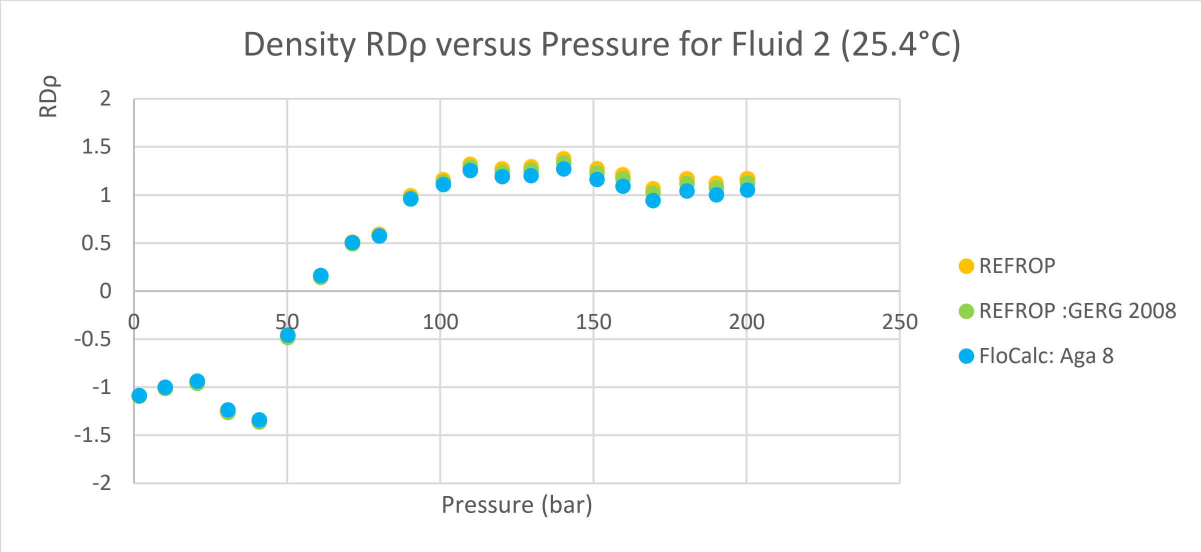

Figure 35: RDp versus Pressure for Fluid 2 (25.4 °C)

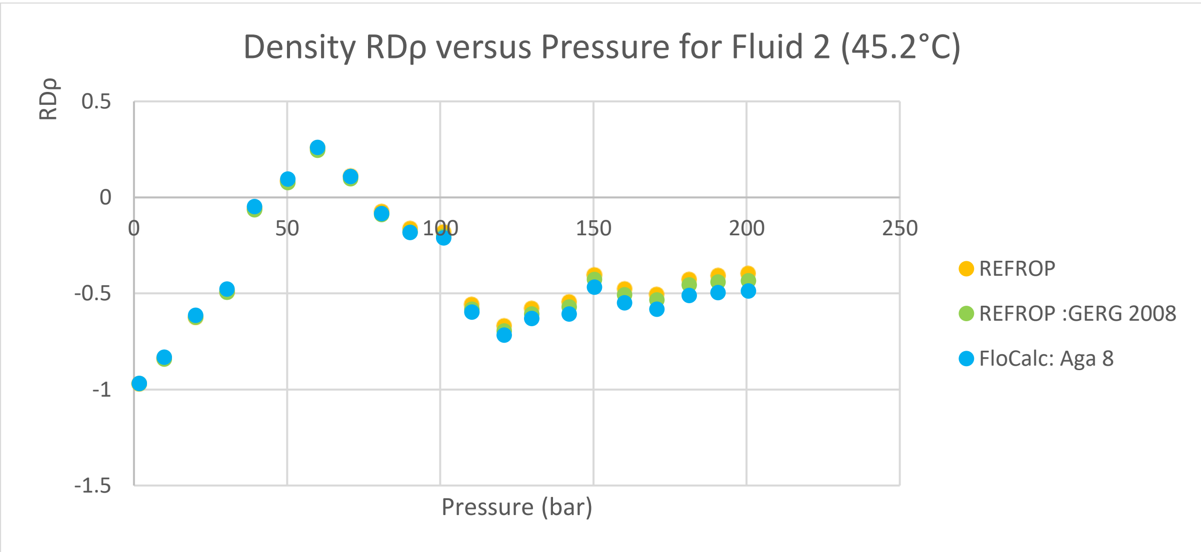

Figure 36: RDp versus Pressure for Fluid 2 (45.2 °C)

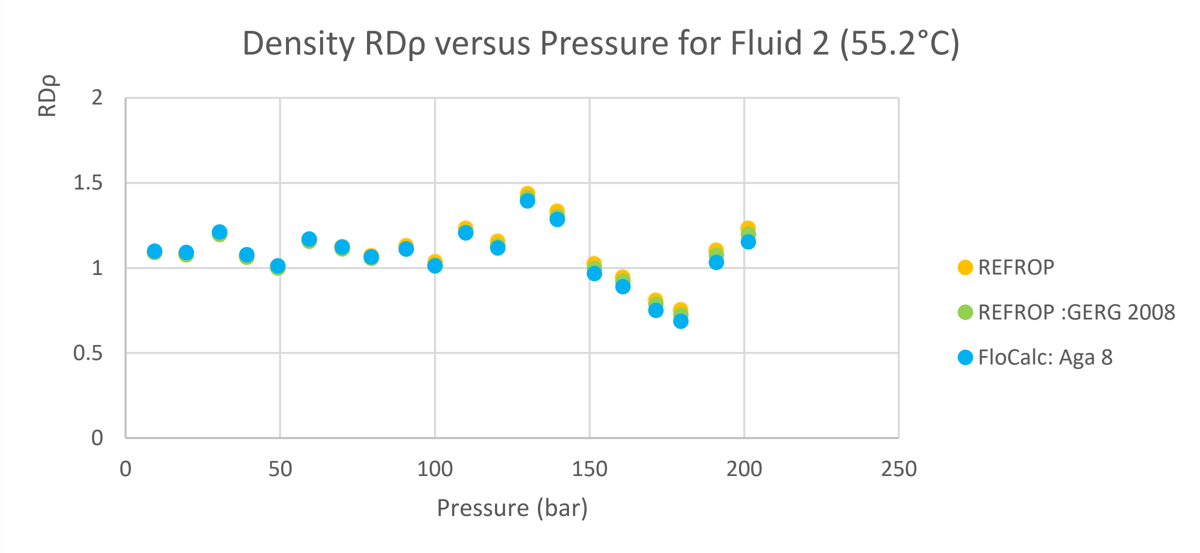

Figure 37: RDp versus Pressure for Fluid 2 (55.2 °C)

EoS	AADp at (up to 200 bar)					
	15.5 °C	25 °C	35 °C	45°C	55°C	65°C
REFPROP	1.158	1.039	**1.125**	**0.420**	1.100	**0.706**
GERG	1.128	1.015	1.150	0.436	1.082	0.723
AGA 8	**1.097**	**0.980**	1.169	0.454	**1.073**	0.726

Table 27: Fluid 2 AADp for each EoS

7.1.4 Fluid 3 (10% H_2 + NG)

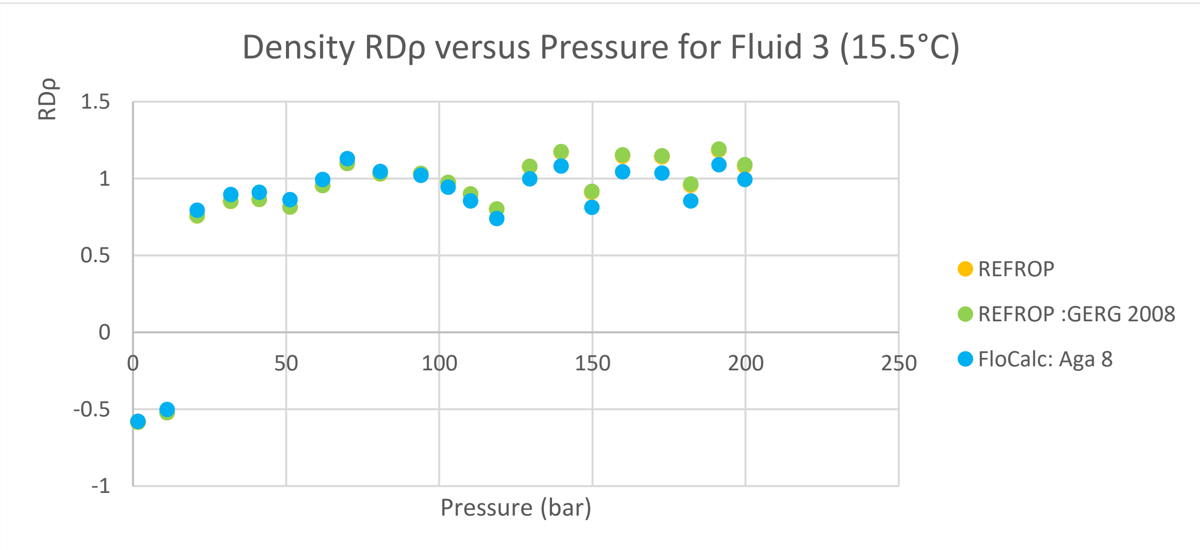

Figure 38: RDp versus Pressure for Fluid 3 (15.5 °C)

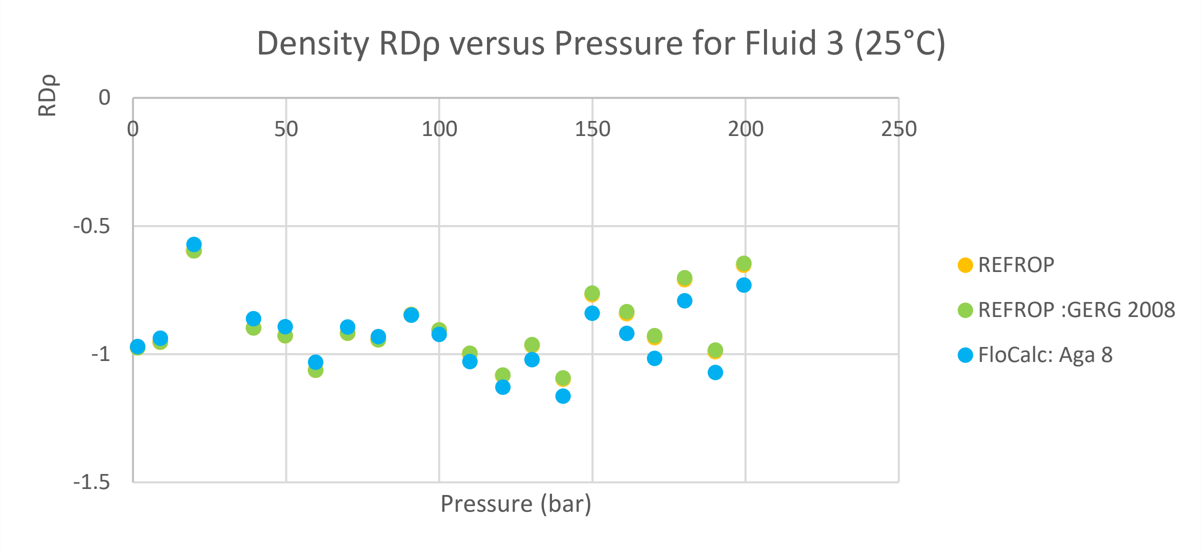

Figure 39: RDρ versus Pressure for Fluid 3 (25 °C)

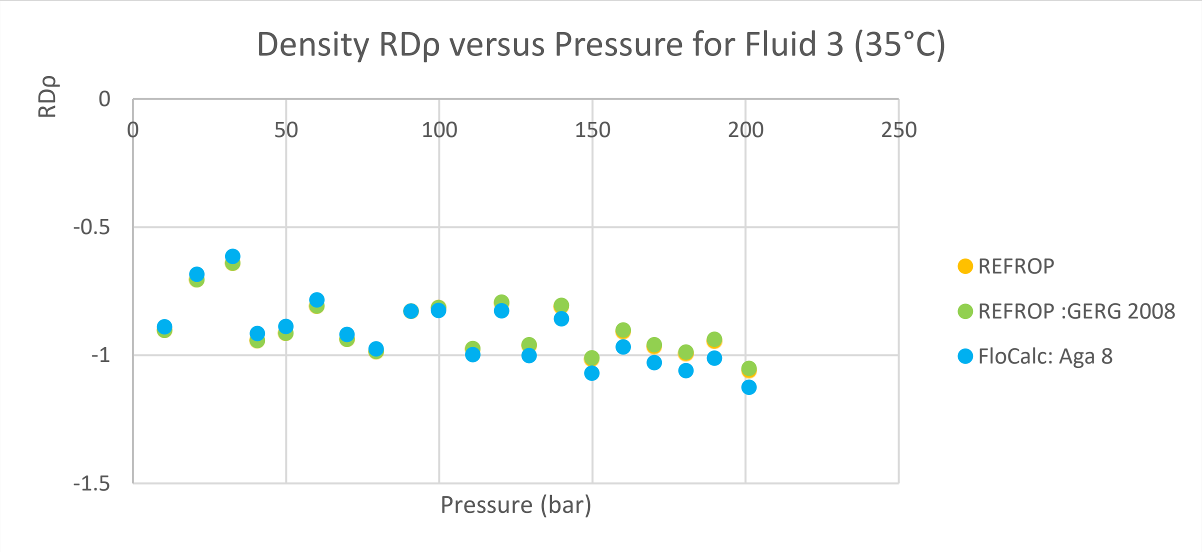

Figure 40: RDρ versus Pressure for Fluid 3 (35 °C)

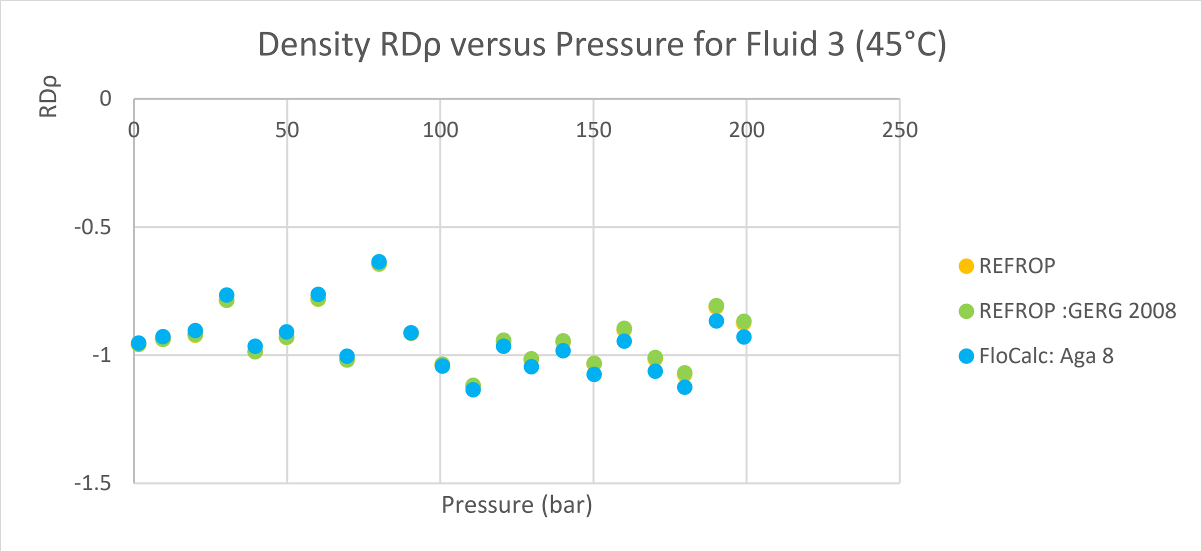

Figure 41: RDρ versus Pressure for Fluid 3 (45 °C)

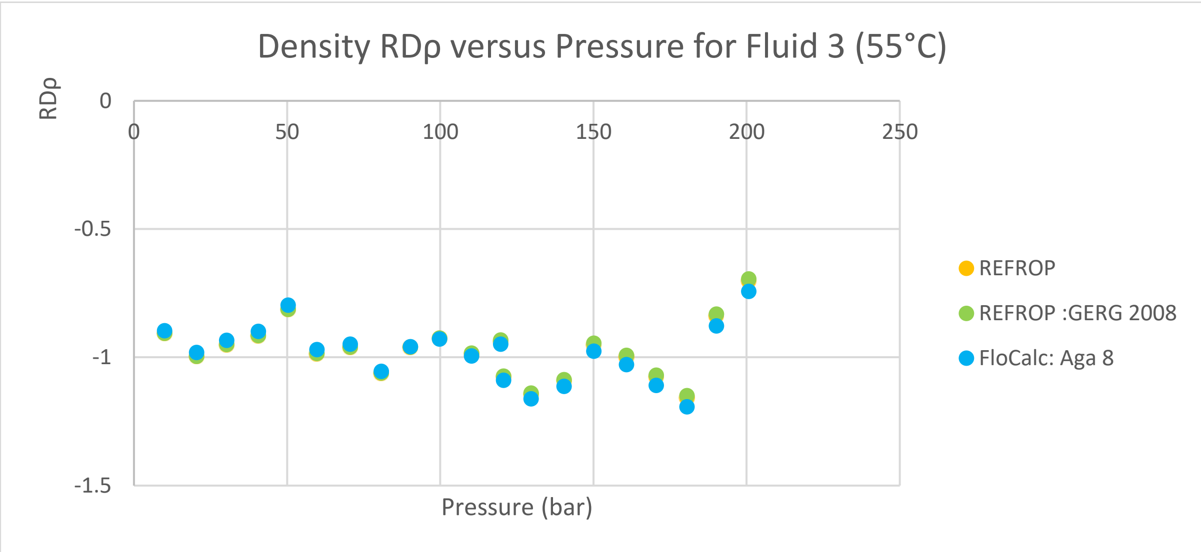

Figure 42: RDρ versus Pressure for Fluid 3 (55 °C)

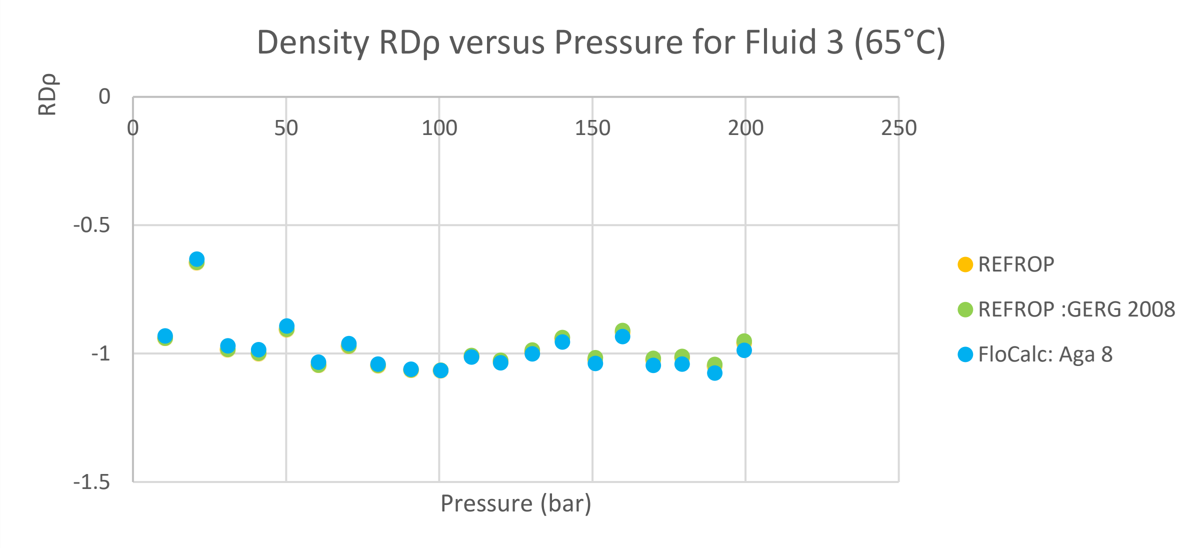

Figure 43: RDρ versus Pressure for Fluid 3 (65 °C)

EoS	AADρ at (10- 200 bar)					
	15.5 °C	25 °C	35 °C	45°C	55°C	65°C
REFPROP	0.963	0.900	0.896	0.936	0.973	0.982
GERG	0.966	**0.896**	**0.893**	**0.932**	**0.969**	**0.978**
AGA 8	**0.930**	0.926	0.913	0.948	0.981	0.985

Table 28: Fluid 3 AADρ for each EoS

7.1.5 Fluid 3a (10% H_2 + NG)

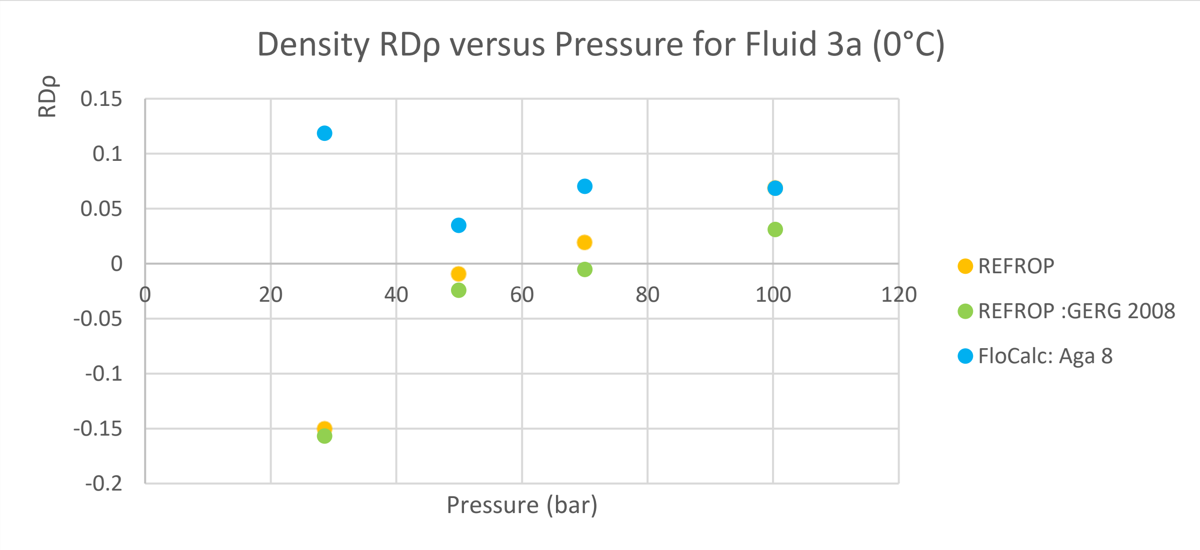

Figure 44: RDρ versus Pressure for Fluid 3a (0°C)

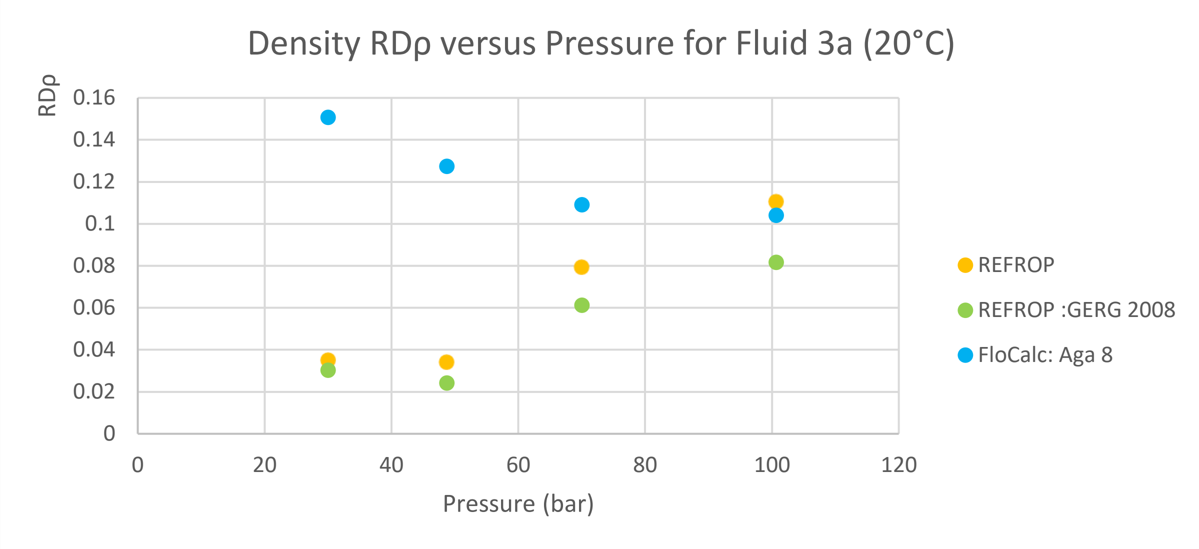

Figure 45: RDp versus Pressure for Fluid 3a (20°C)

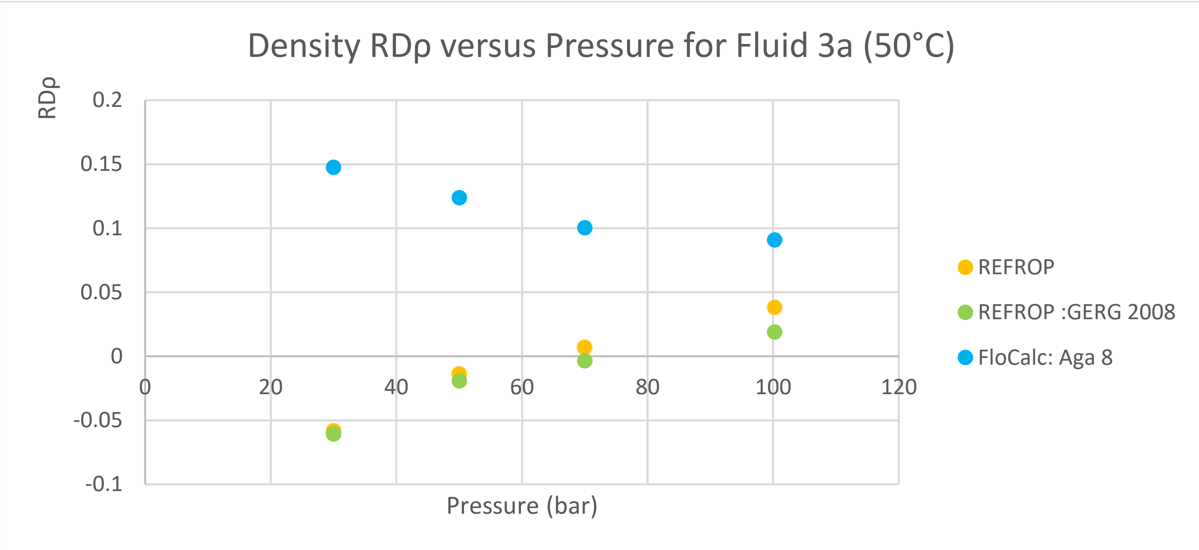

Figure 46: RDp versus Pressure for Fluid 3a (50°C)

EoS	AADp at (30 up to 100 bar)		
	0 °C	20°C	50 °C
REFPROP	0.062	0.065	0.029
GERG	0.054	**0.049**	0.026
AGA 8	**0.040**	0.062	**0.020**

Table 29: Fluid 3a AADp for each EoS

7.1.6 Fluid 4 (15% H_2 + NG)

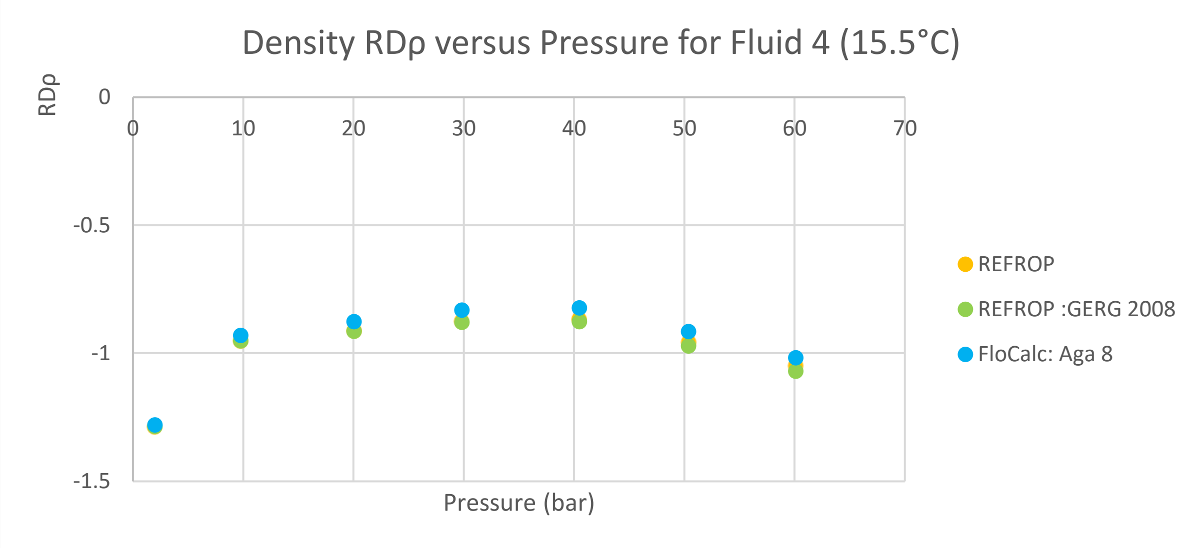

Figure 47: RDρ versus Pressure for Fluid 4 (15.5°C)

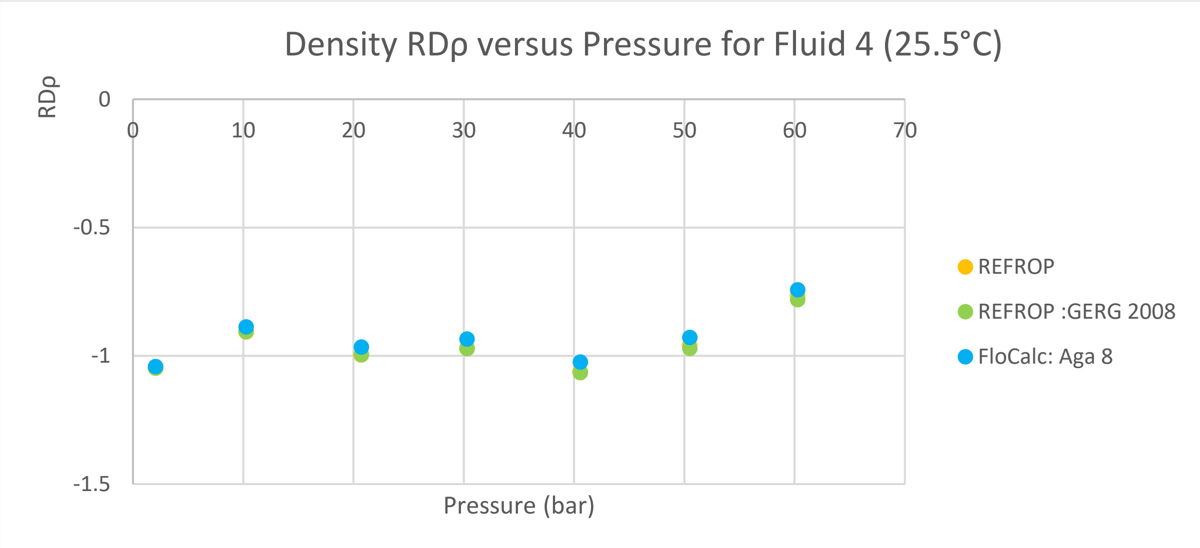

Figure 48: RDρ versus Pressure for Fluid 4 (25.5°C)

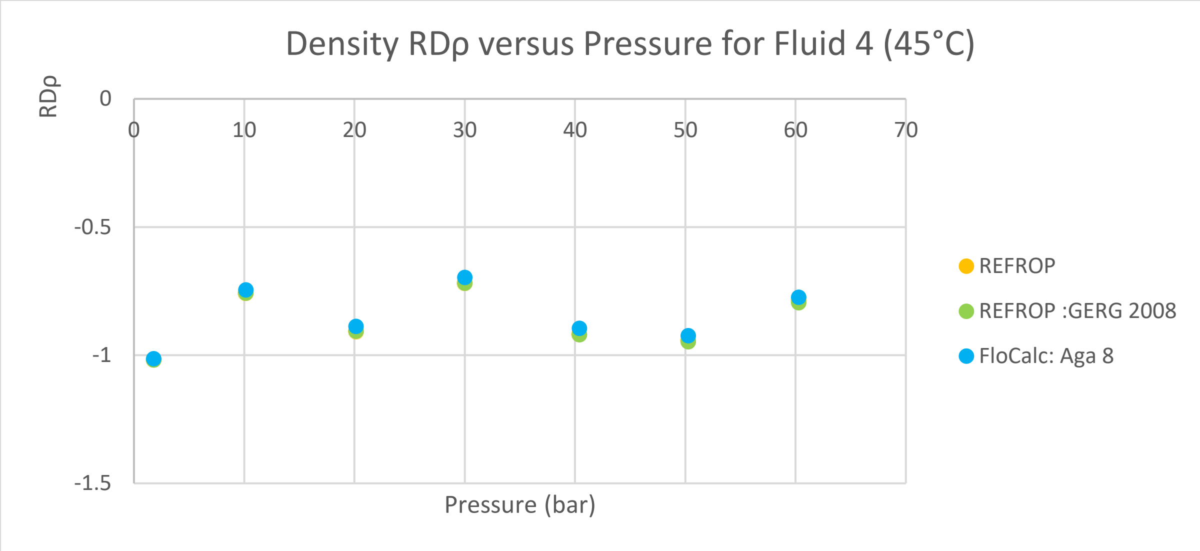

Figure 49: RDρ versus Pressure for Fluid 4 (45°C)

EoS	AADρ at (1- 60 bar)		
	15.5 °C	25.5 °C	45°C
REFPROP	0.986	0.958	0.864
GERG	0.993	0.964	0.866
AGA 8	**0.954**	**0.933**	**0.848**

Table 30: Fluid 4 AADρ for each EoS

7.1.7 Fluid 4a (15% H_2 + NG)

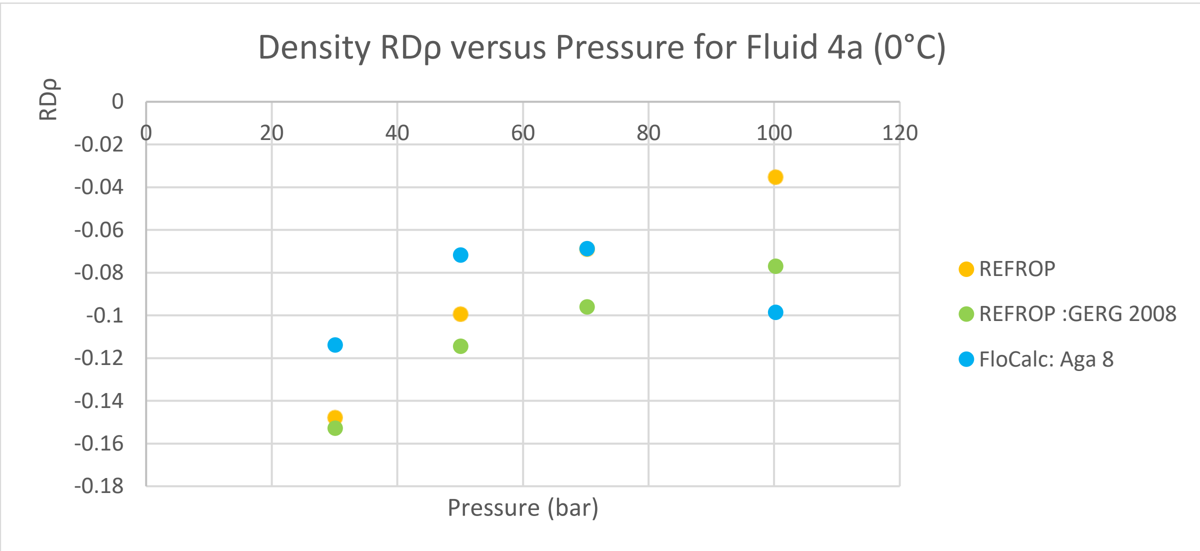

Figure 50: RDρ versus Pressure for Fluid 4a (0°C)

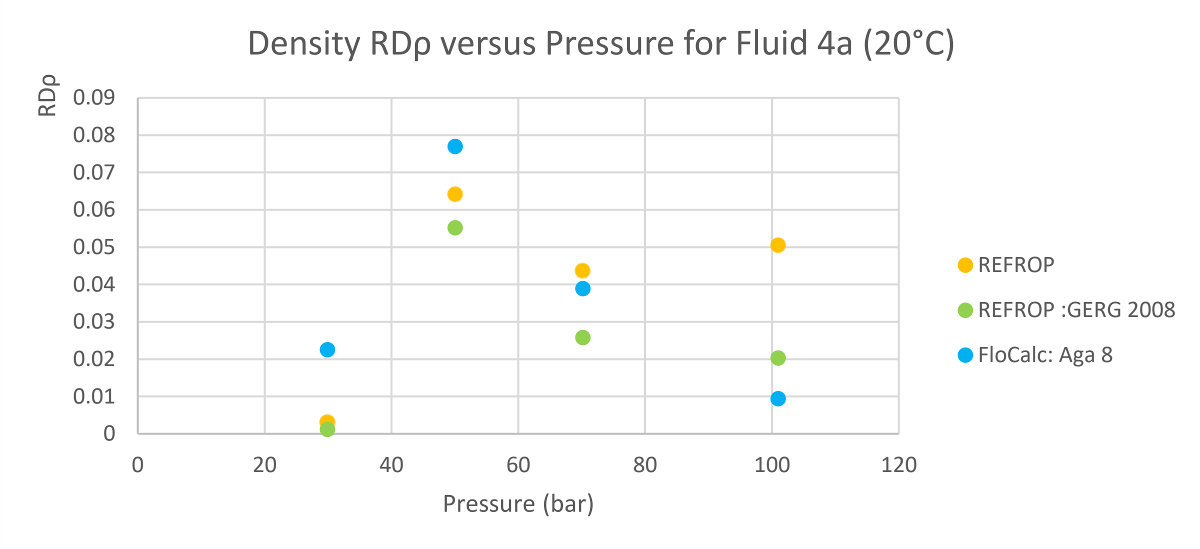

Figure 51: RDp versus Pressure for Fluid 4a (20°C)

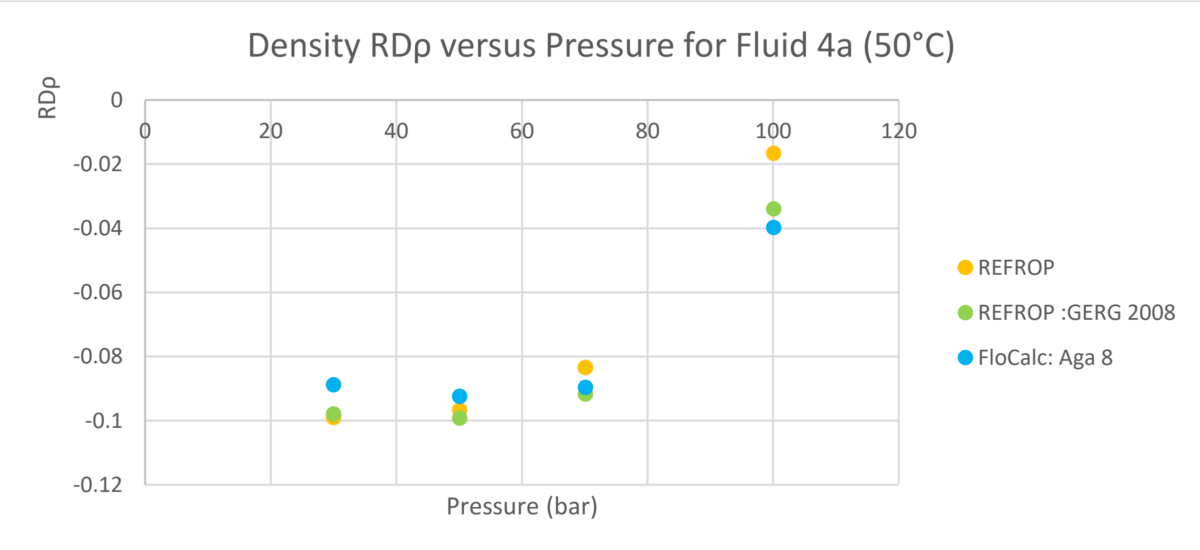

Figure 52: RDp versus Pressure for Fluid 4a (50°C)

EoS	AADp at (30 up to 100 bar)		
	0 °C	20°C	50 °C
REFPROP	**0.088**	0.040	**0.074**
GERG	0.110	**0.026**	0.081
AGA 8	0.088	0.037	0.078

Table 31: Fluid 4a AADp for each EoS

7.1.8 Fluid 5 (20% H_2 + NG)

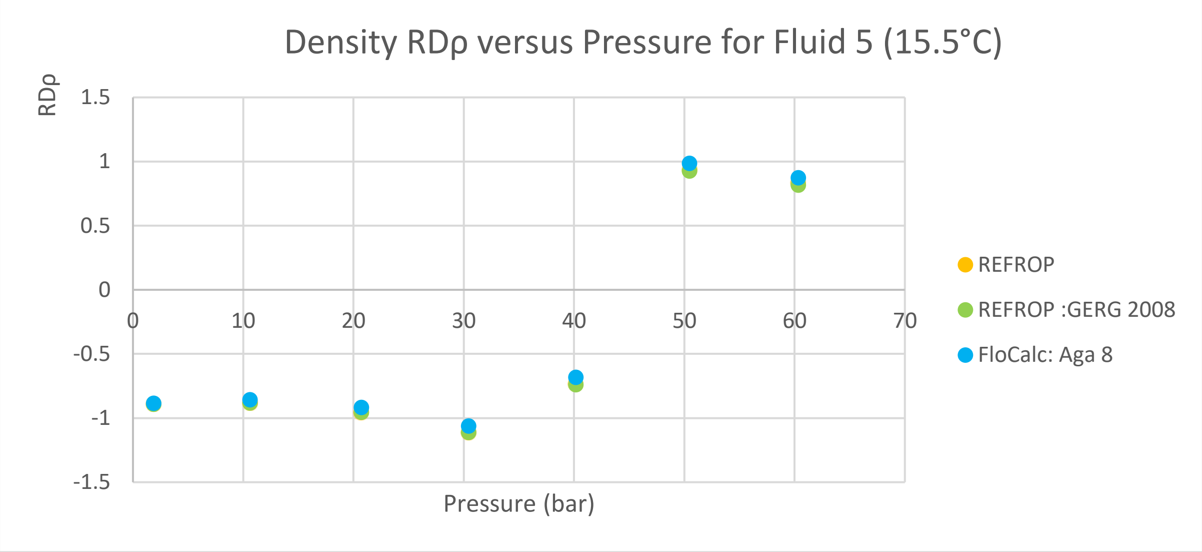

Figure 53: RDρ versus Pressure for Fluid 5 (15.5°C)

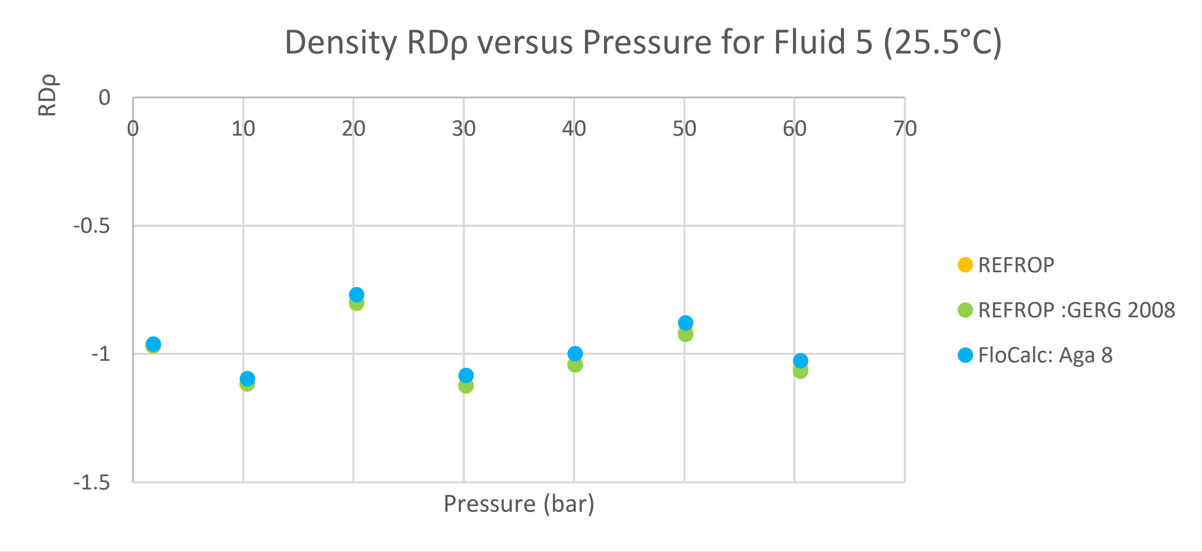

Figure 54: RDρ versus Pressure for Fluid 5 (25.5°C)

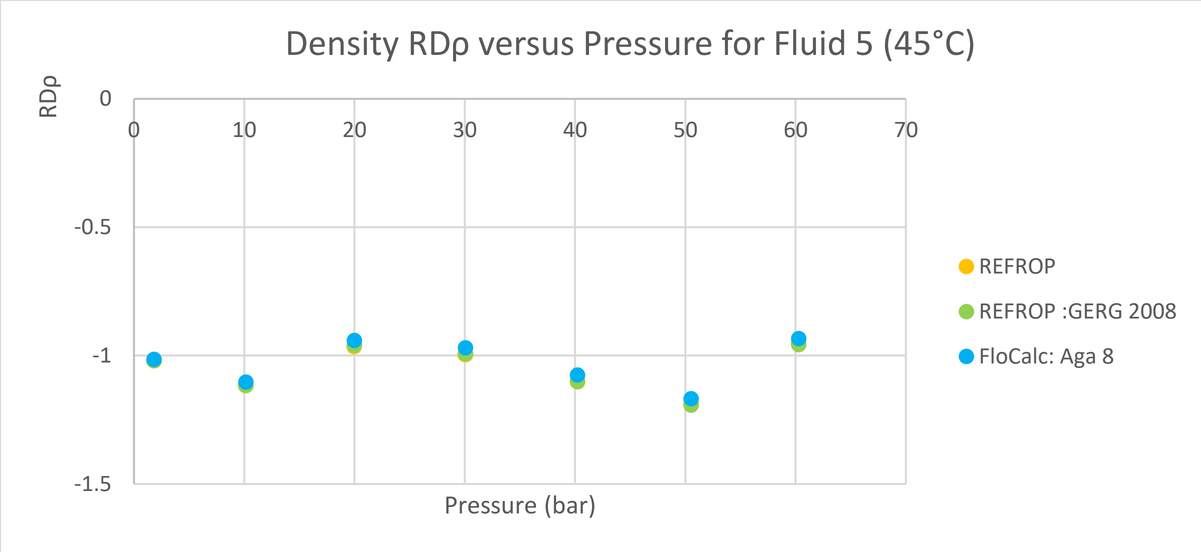

Figure 55: RDρ versus Pressure for Fluid 5 (45°C) 4

EoS	AADρ at (1- 60 bar)		
	15.5 °C	25.5 °C	45°C
REFPROP	0.907	1.004	1.049
GERG	0.903	1.006	1.048
AGA 8	**0.895**	**0.974**	**1.029**

Table 32: Fluid 5 AADρ for each EoS

7.1.9 Fluid 5a (20% H_2 + NG)

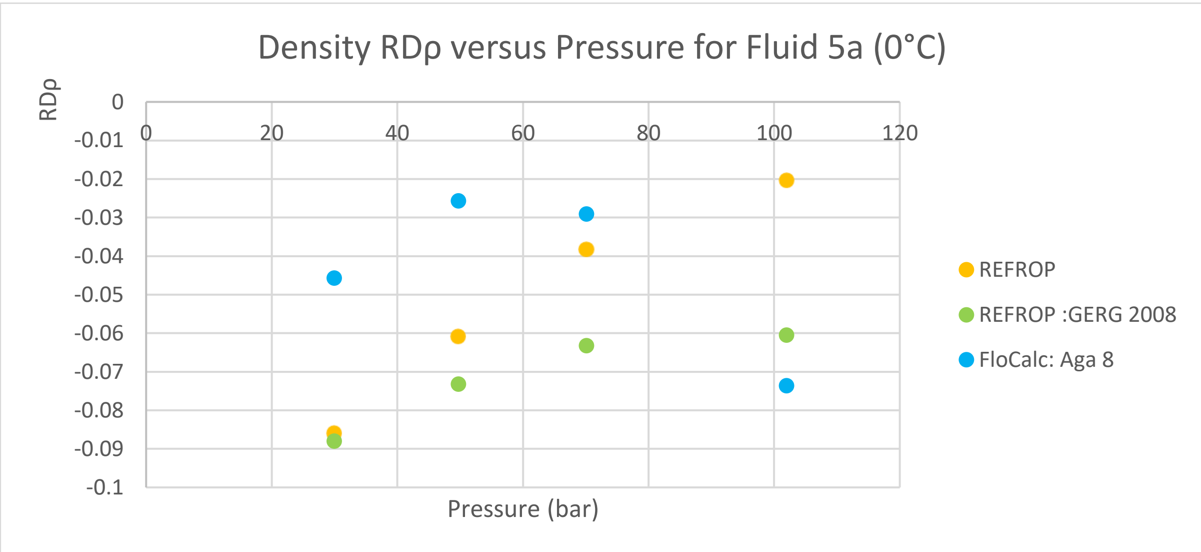

Figure 56: RDρ versus Pressure for Fluid 5a (0°C)

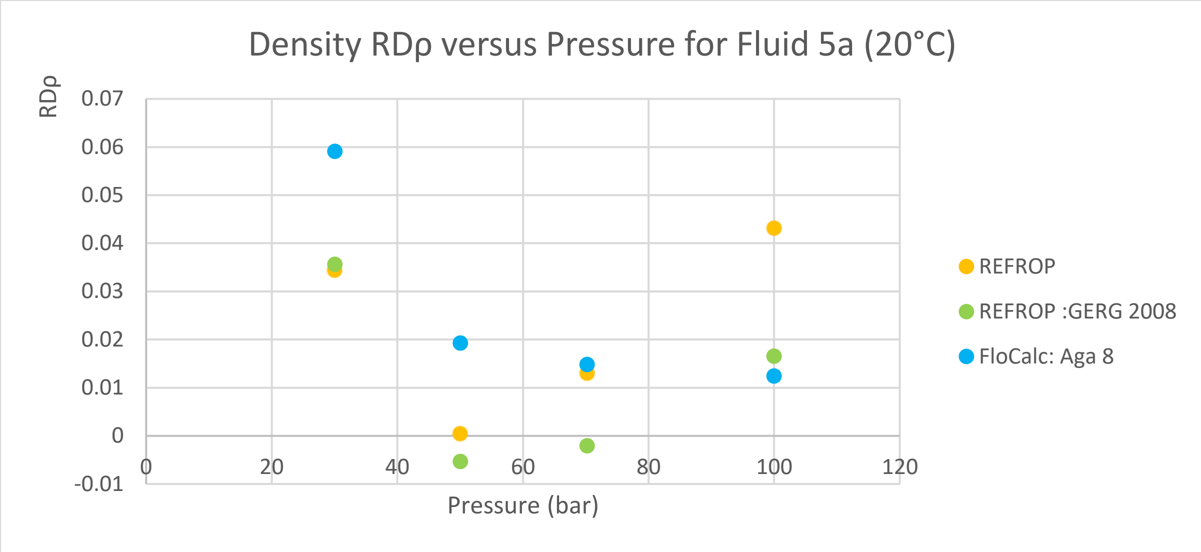

Figure 57: RDp versus Pressure for Fluid 5a (20°C)

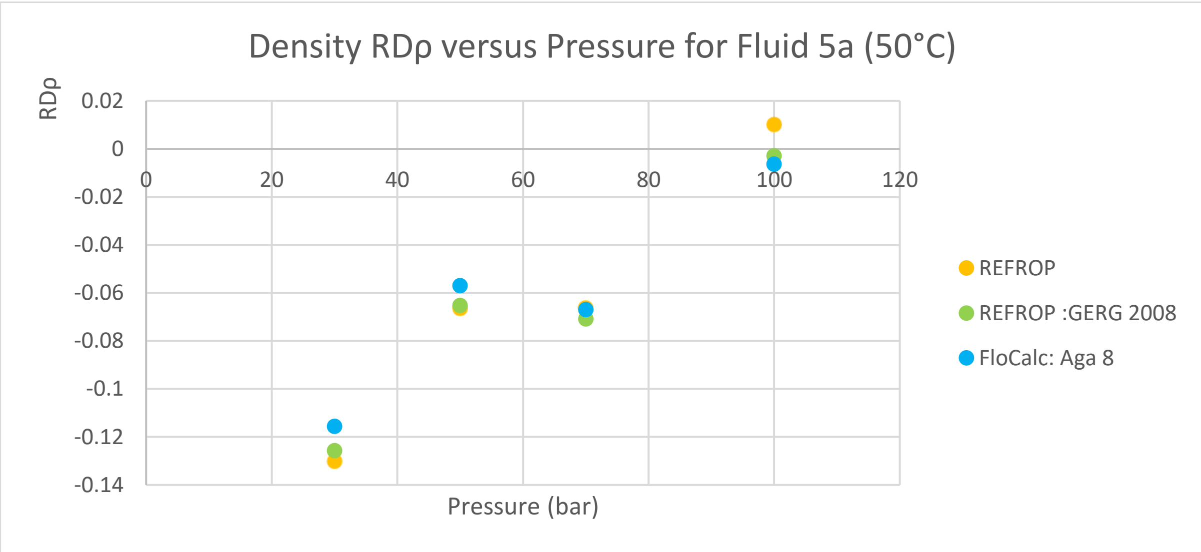

Figure 58: RDp versus Pressure for Fluid 5a (50°C)

EoS	**AADp at (30 up to 100 bar)**		
	0 °C	20°C	50 °C
REFPROP	0.051	0.023	0.068
GERG	0.071	**0.015**	0.066
AGA 8	**0.043**	0.026	**0.061**

Table 33: Fluid 5a AADp for each EoS

7.1.10 Fluid 6 (5% H_2 + 95% CH_4)

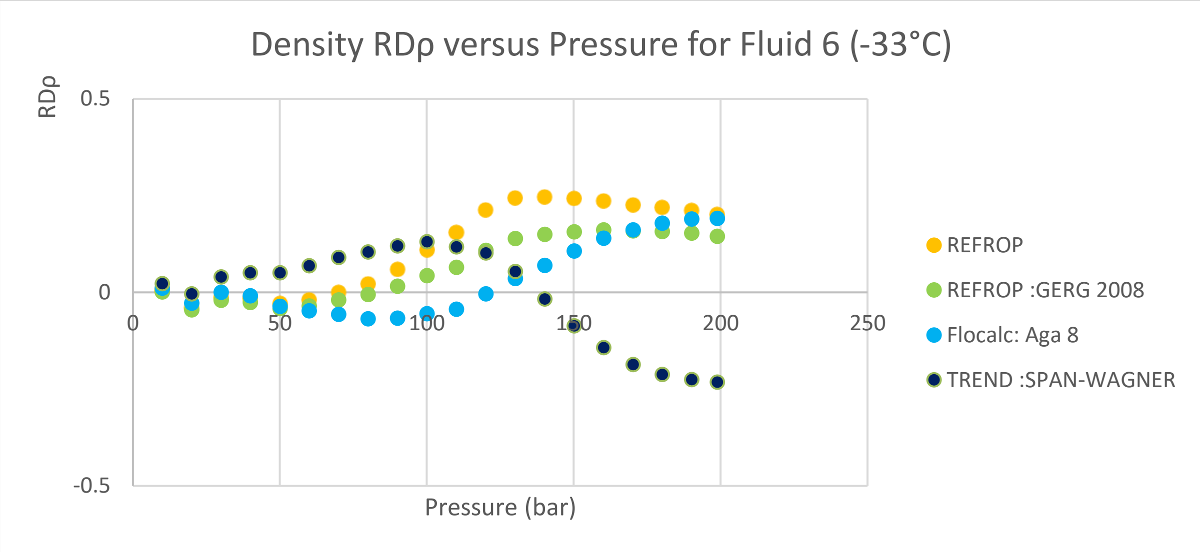

Figure 59: RDρ versus Pressure for Fluid 6 (-33°C)

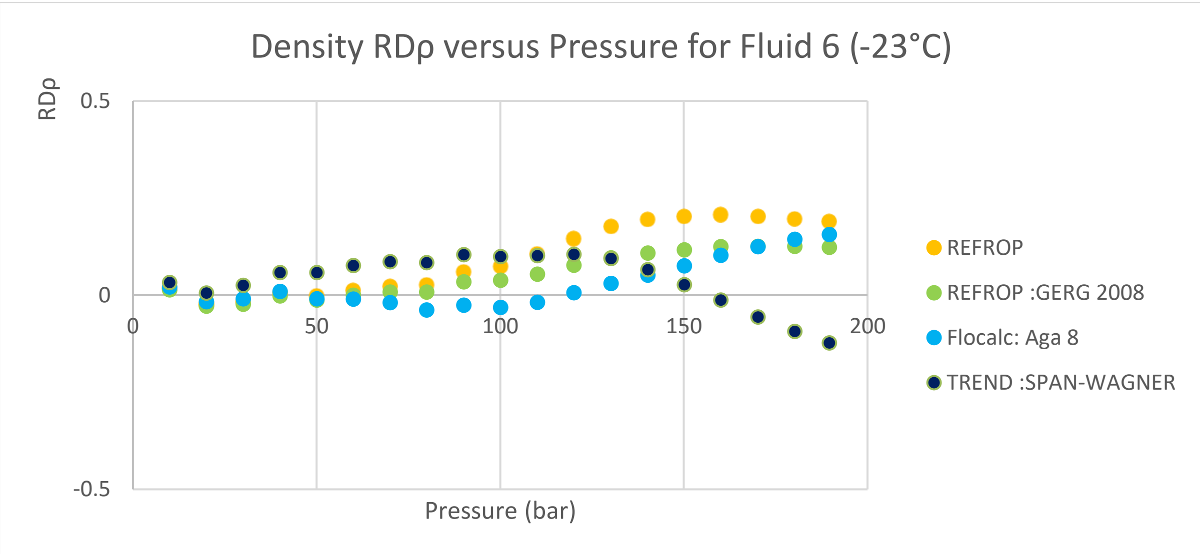

Figure 60: RDρ versus Pressure for Fluid 6 (-23°C)

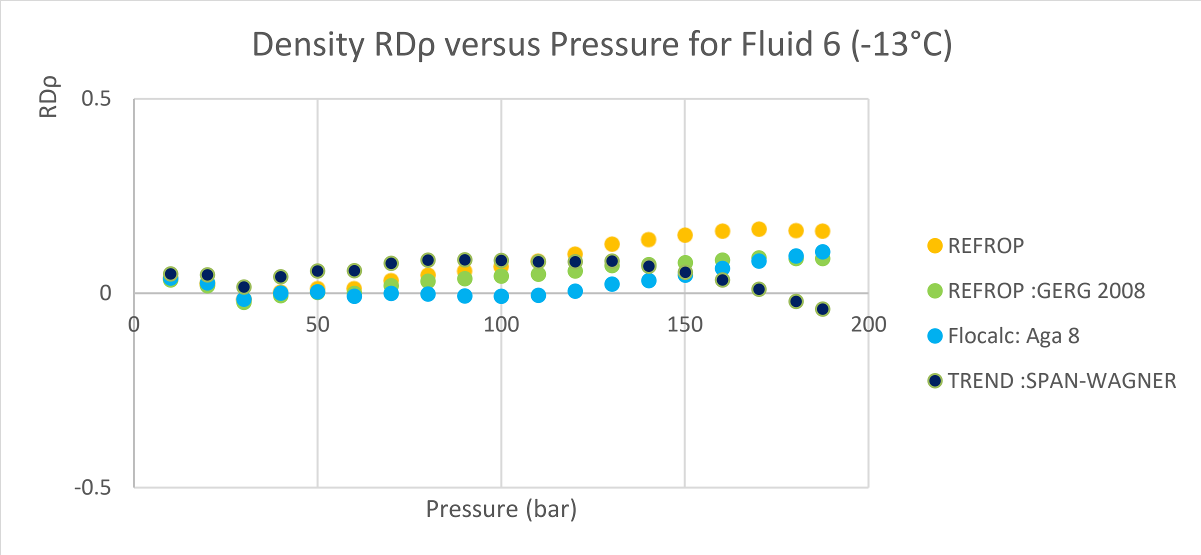

Figure 61: RDρ versus Pressure for Fluid 6 (-13°C)

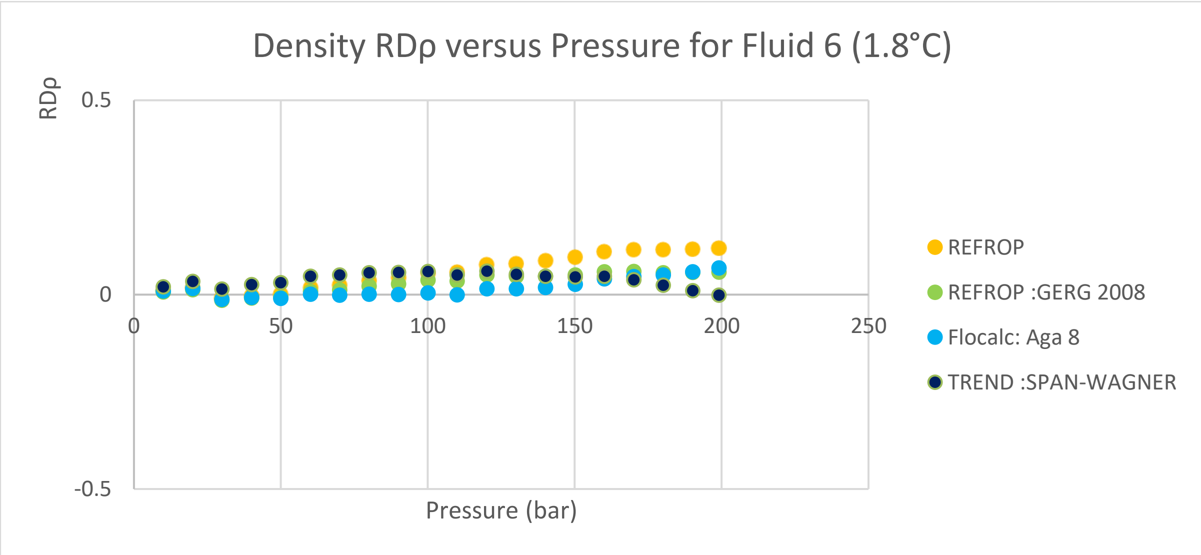

Figure 62: RDρ versus Pressure for Fluid 6 (1.8°C)

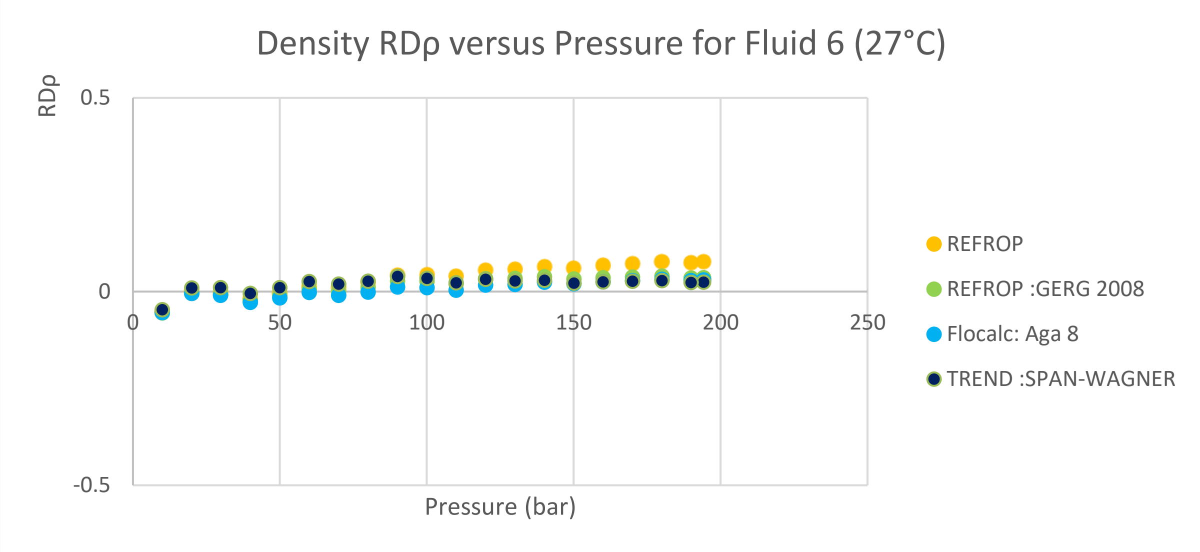

Figure 63: RDρ versus Pressure for Fluid 6 (27°C)

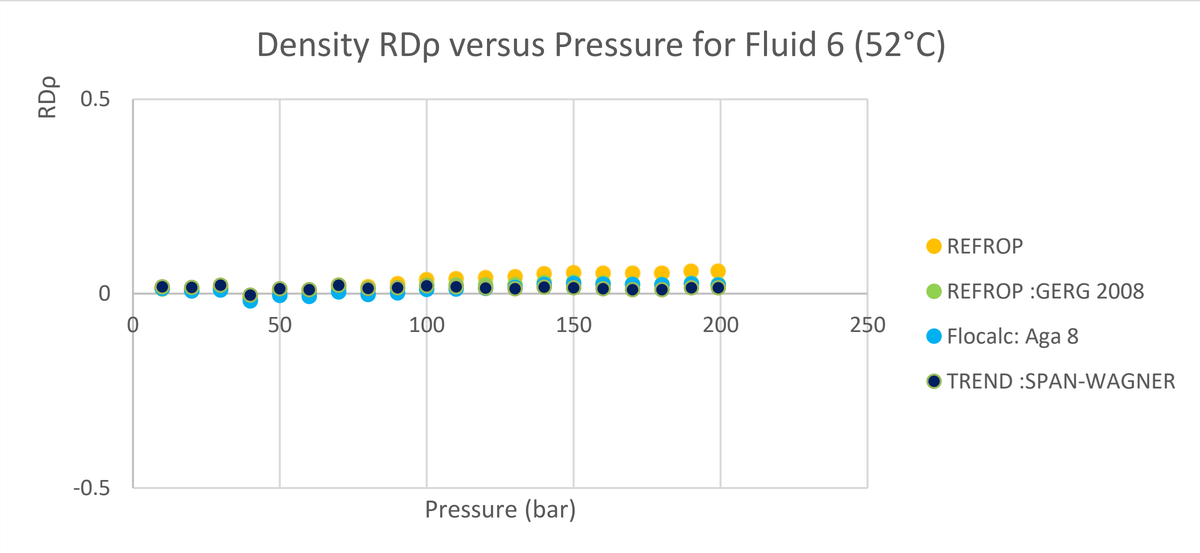

Figure 64: RDρ versus Pressure for Fluid 6 (52°C)

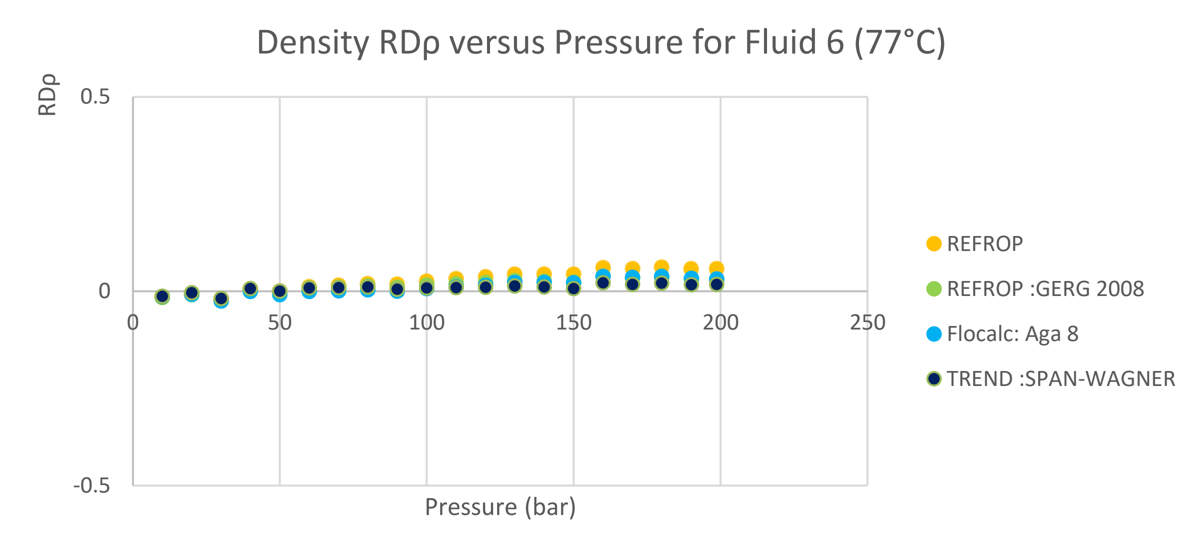

Figure 65: RDρ versus Pressure for Fluid 6 (77°C)

EoS	AADρ at (10 - 200 bar)						
	-33 °C	-23 °C	-13 °C	2°C	27°C	52°C	77°C
REFPROP	0.125	0.099	0.081	0.060	0.043	0.033	0.031
GERG	0.082	0.059	0.047	0.034	0.026	0.018	0.020
Span - Wagner	0.103	0.069	0.057	0.039	0.024	0.015	**0.012**
AGA 8	**0.075**	**0.047**	**0.030**	**0.020**	**0.019**	**0.014**	0.017
PR	2.639	2.634	2.623	2.567	2.402	2.213	2.019
SRK	2.836	2.367	2.096	1.915	1.586	1.383	1.249
PC-SAFT	1.389	1.455	1.534	1.526	1.475	1.338	1.187

Table 34: Fluid 6 AADρ for each EoS

7.1.11 Fluid 7 (8.58% H_2 + 91.42% CH_4)

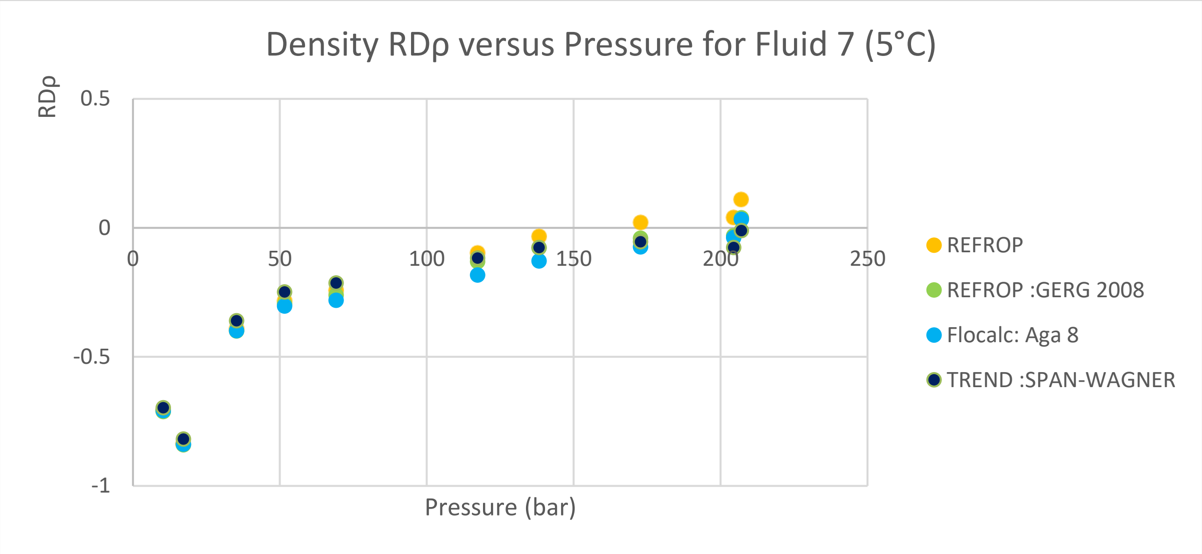

Figure 66: RDρ versus Pressure for Fluid 7 (5°C)

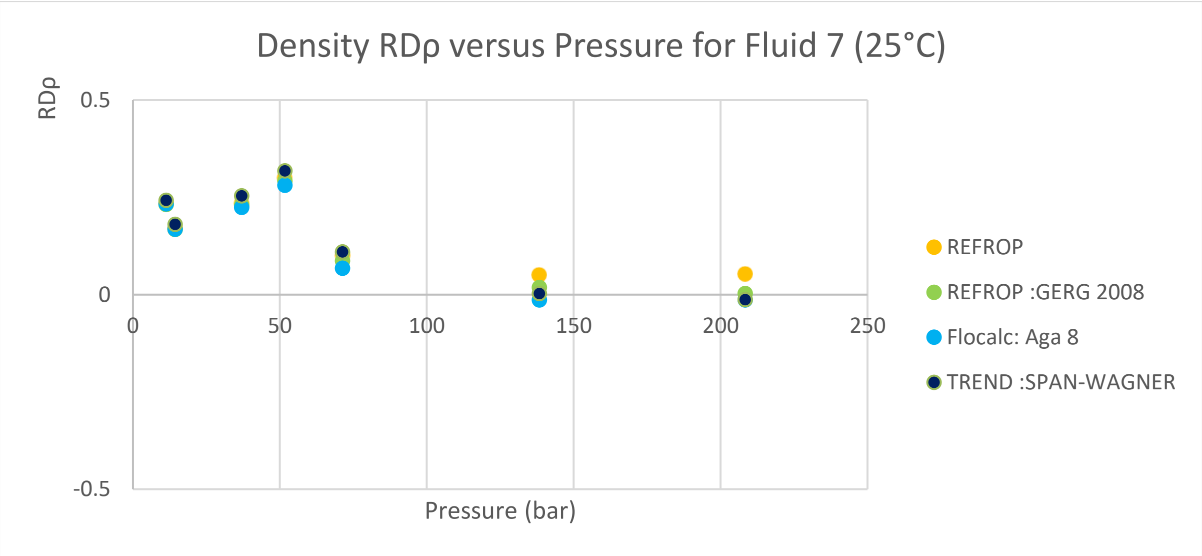

Figure 67: RDρ versus Pressure for Fluid 7 (25°C)

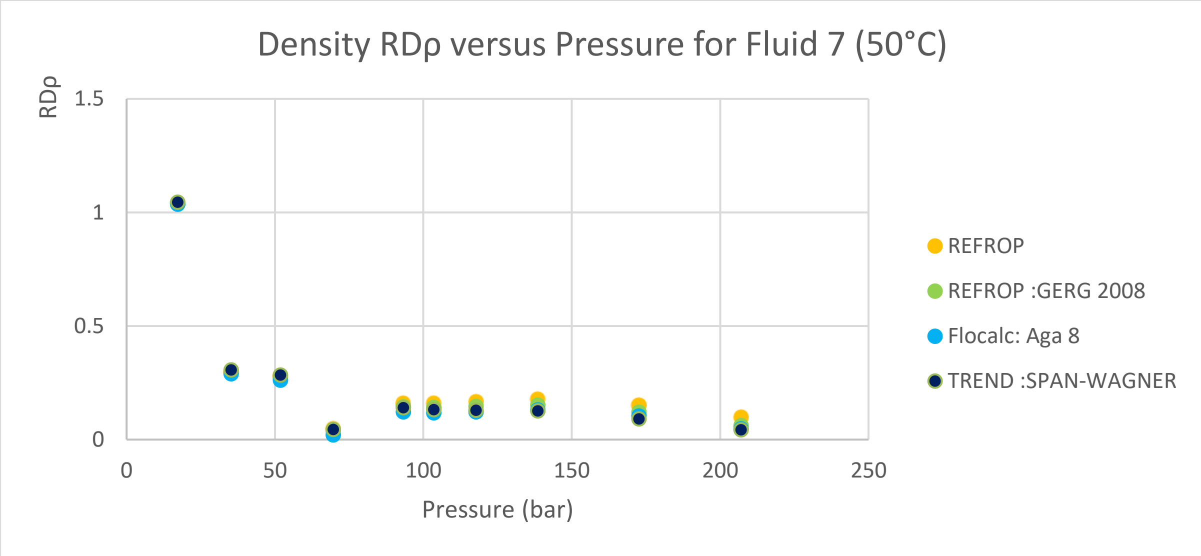

Figure 68: RDp versus Pressure for Fluid 7 (50°C)

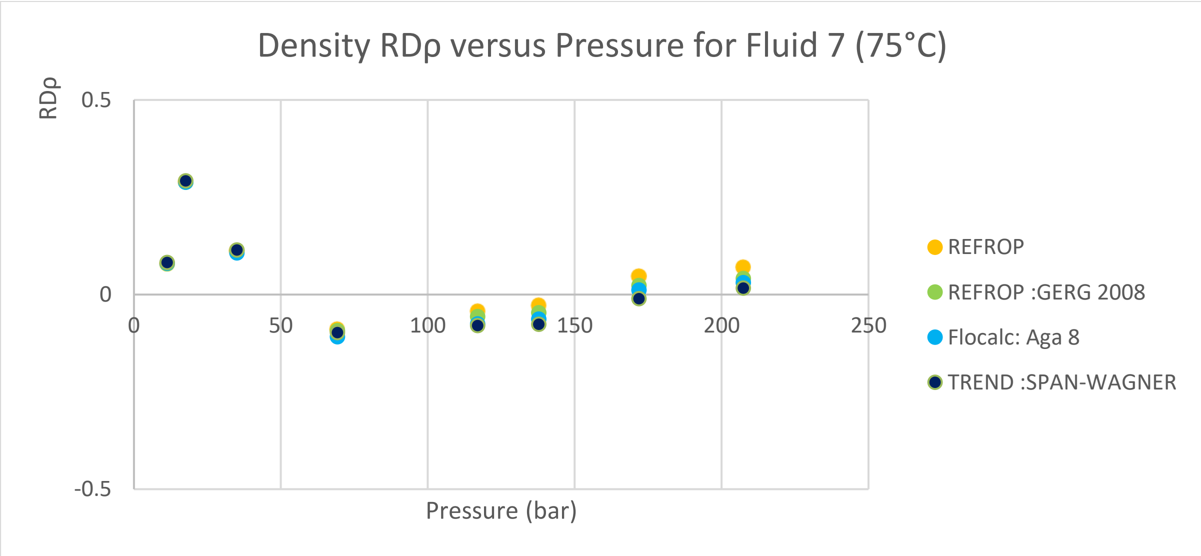

Figure 69: RDp versus Pressure for Fluid 7 (75°C)

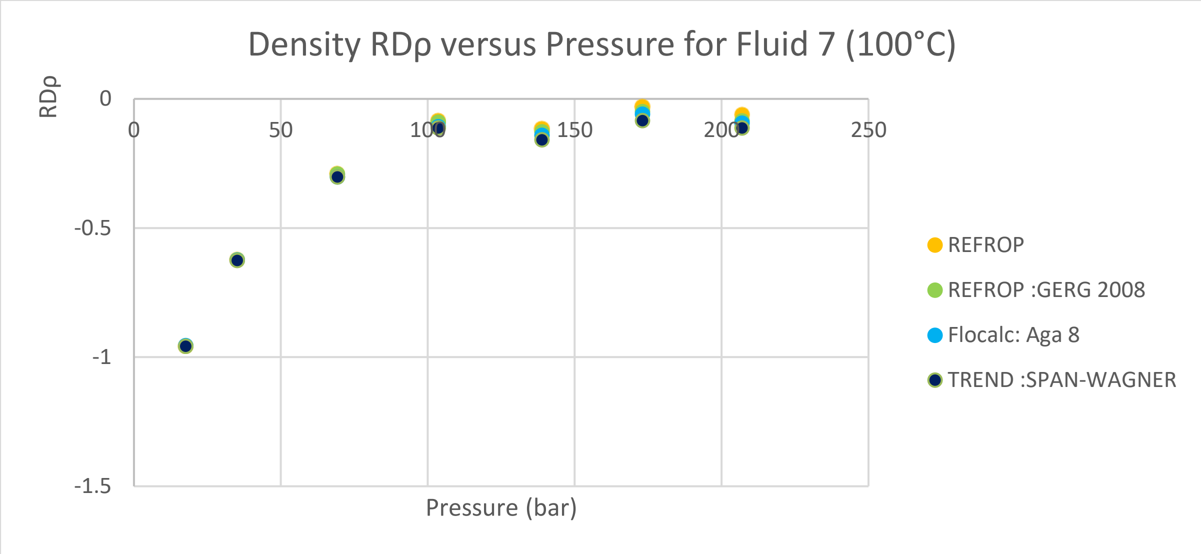

Figure 70: RDρ versus Pressure for Fluid 7 (100°C)

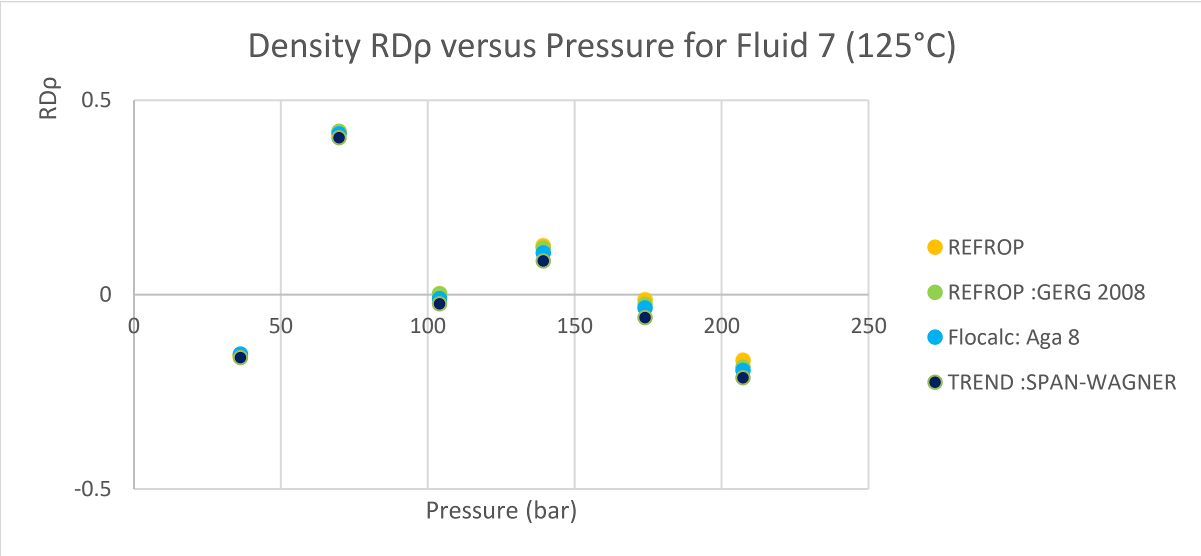

Figure 71: RDρ versus Pressure for Fluid 7 (125°C)

EoS	AADρ at (10 - 200 bar)			AADρ at (20 - 200 bar)	
	5 °C	25 °C	75°C	50 °C	100°C
REFPROP	0.276	0.163	0.095	0.258	**0.309**
GERG	0.282	0.147	**0.092**	0.241	0.318
Span - Wagner	**0.267**	0.160	0.096	0.235	0.336
AGA 8	0.298	**0.143**	0.096	**0.226**	0.326
PR	2.233	2.146	1.931	2.566	1.706
SRK	1.823	0.874	1.023	1.112	1.358
PC-SAFT	1.370	1.255	1.144	1.623	1.034

Table 35: Fluid 7 AADρ for each EoS

7.1.12 Fluid 8 (10% H_2 + 90% CH_4)

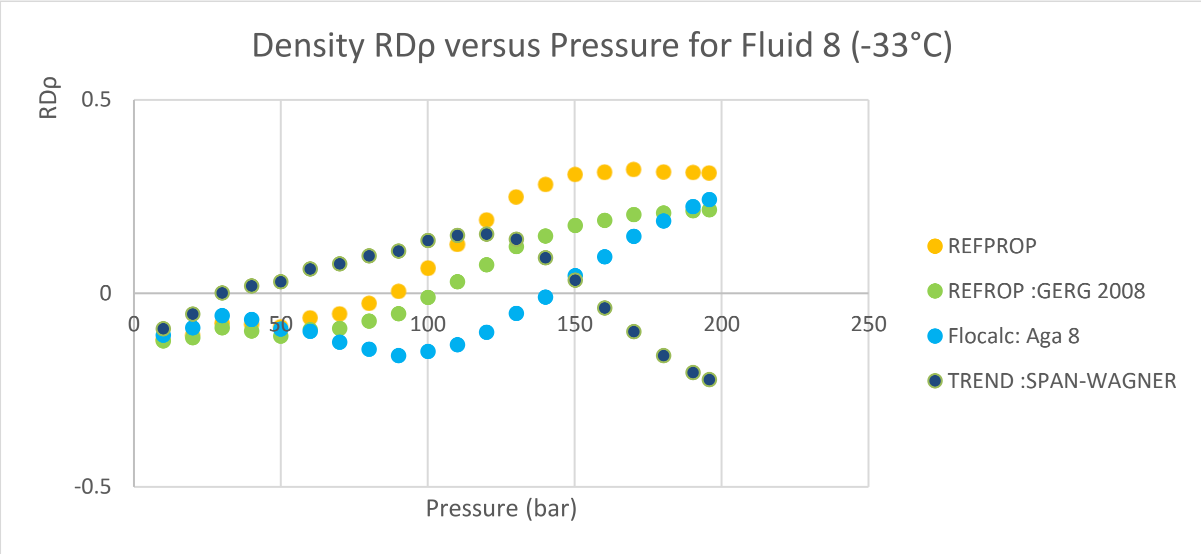

Figure 72: RDρ versus Pressure for Fluid 8 (-33°C)

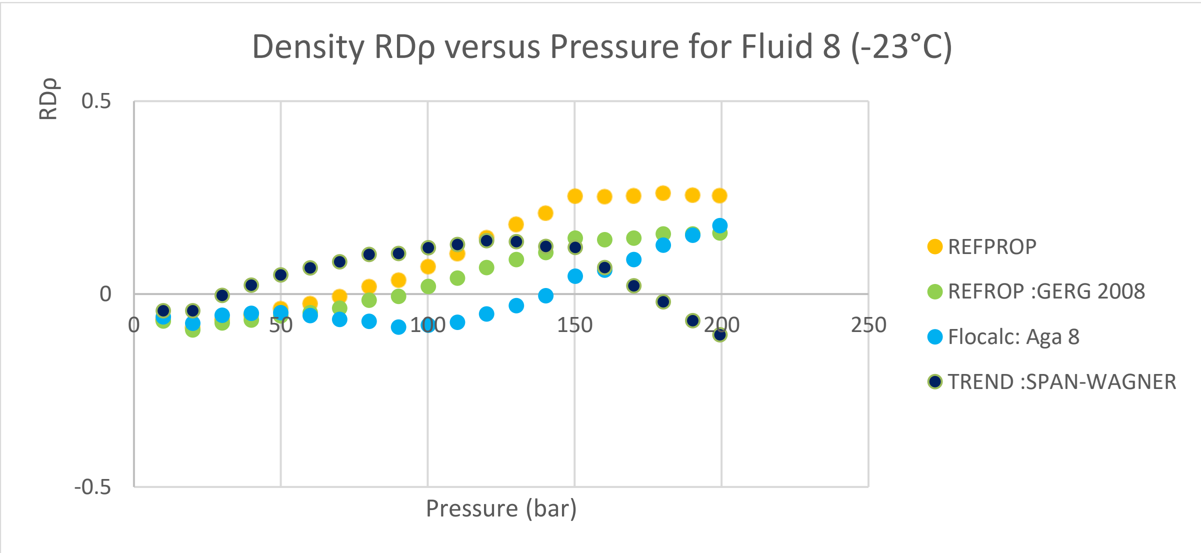

Figure 73: RDρ versus Pressure for Fluid 8 (-23°C)

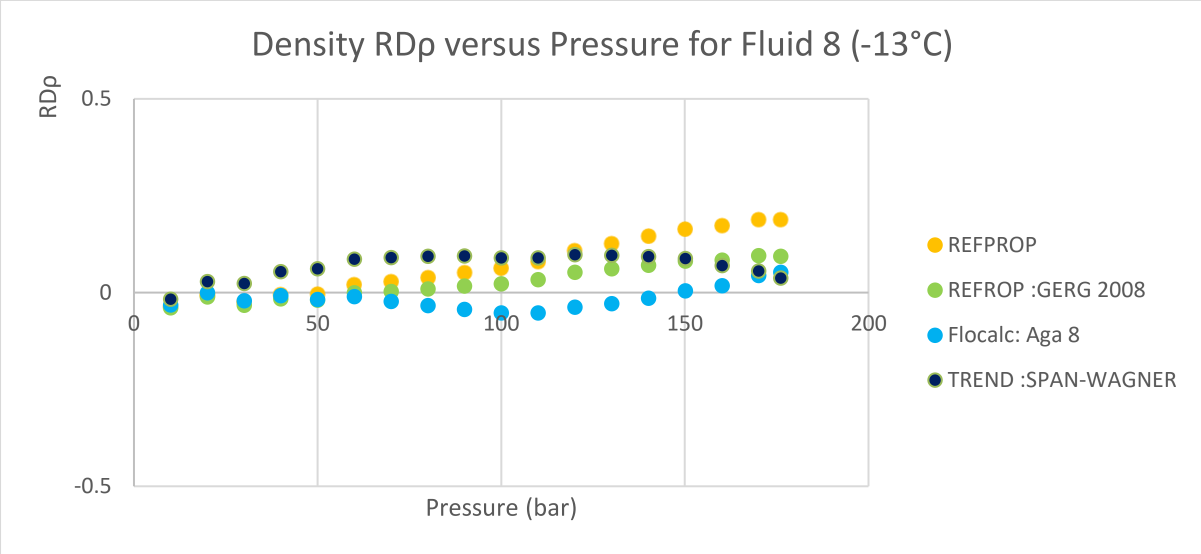

Figure 74: RDρ versus Pressure for Fluid 8 (-13°C)

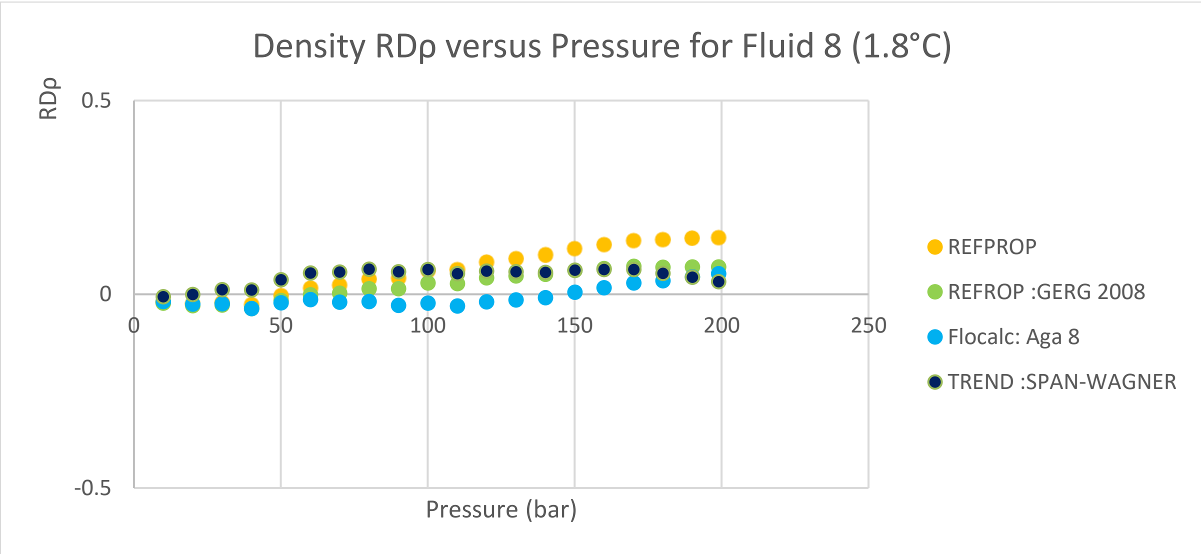

Figure 75: RDρ versus Pressure for Fluid 8 (1.8°C)

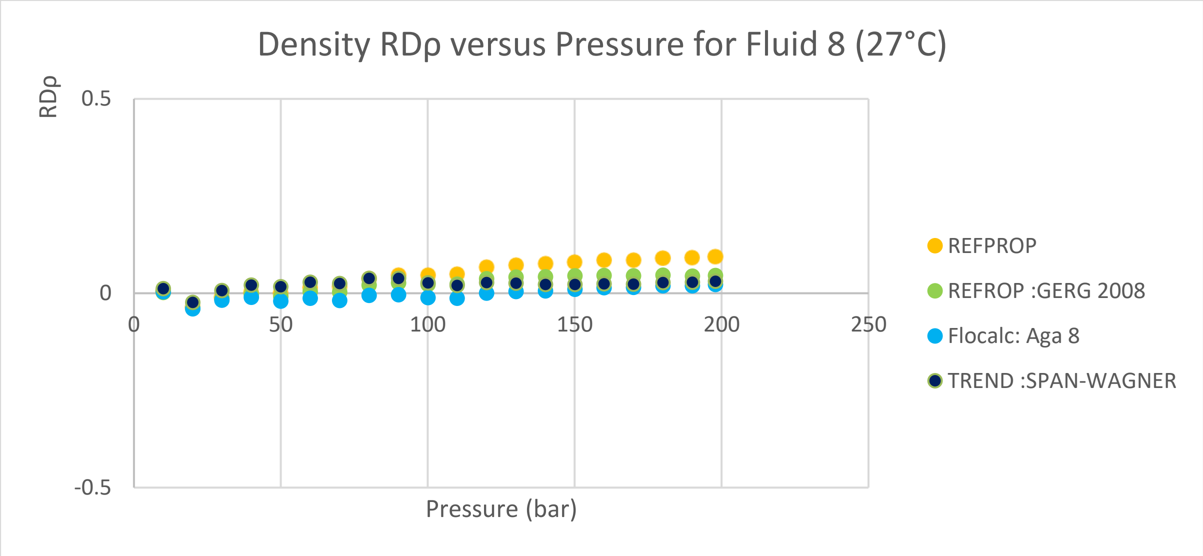

Figure 76: RDp versus Pressure for Fluid 8 (27°C)

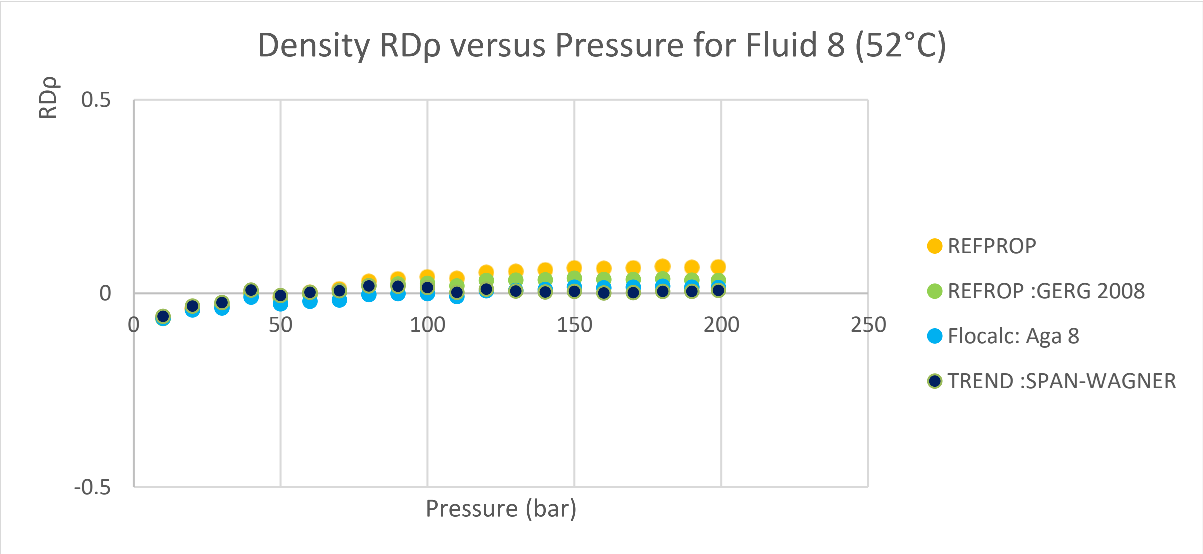

Figure 77: RDp versus Pressure for Fluid 8 (52°C)

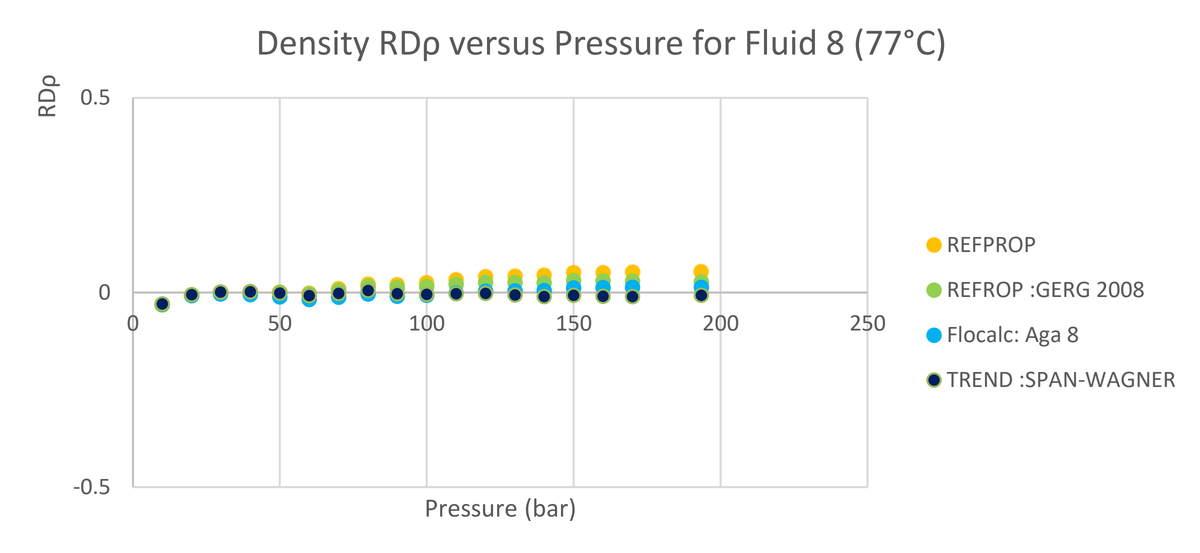

Figure 78: RDρ versus Pressure for Fluid 8 (77°C)

EoS	AADρ at (10 - 200 bar)						
	-33 °C	-23 °C	-13 °C	2°C	27°C	52°C	77°C
REFPROP	0.170	0.139	0.080	0.072	0.050	0.044	0.027
GERG	0.121	0.089	0.041	0.039	0.028	0.028	0.017
Span - Wagner	**0.099**	0.083	0.070	0.046	0.025	**0.012**	**0.007**
AGA 8	0.116	**0.077**	**0.027**	**0.024**	**0.013**	0.018	0.010
PR	3.190	3.301	3.036	2.919	2.661	2.400	2.075
SRK	2.158	1.994	1.458	1.482	1.259	1.132	0.931
PC-SAFT	2.142	2.236	2.151	1.932	1.724	1.477	1.194

Table 36: Fluid 8 AADρ for each EoS

7.1.13 Fluid 9a (20% H_2 + 80% CH_4)

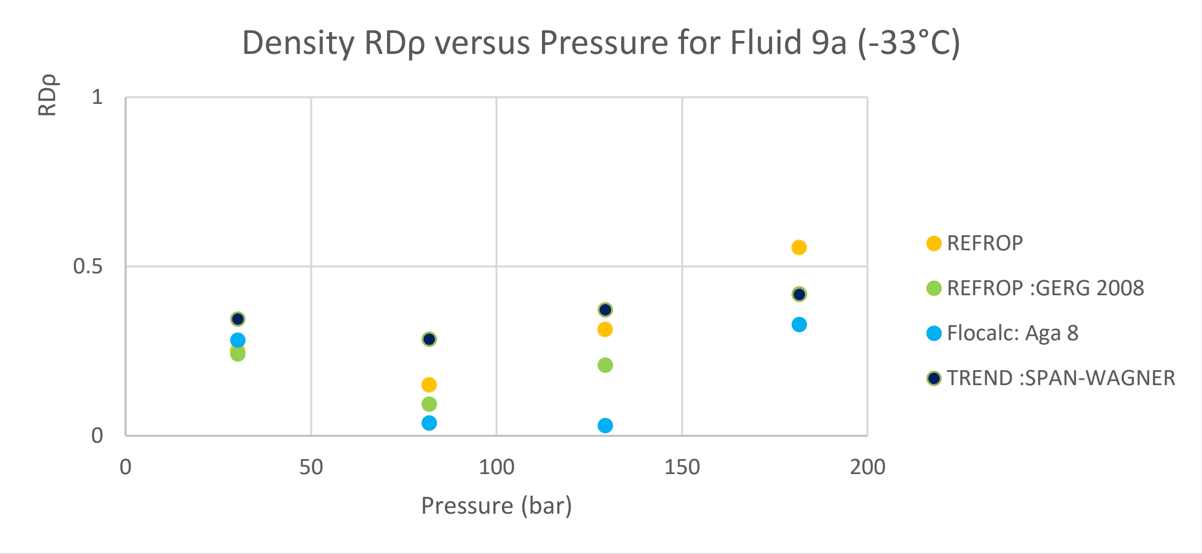

Figure 79: RDρ versus Pressure for Fluid 9a (-33°C)

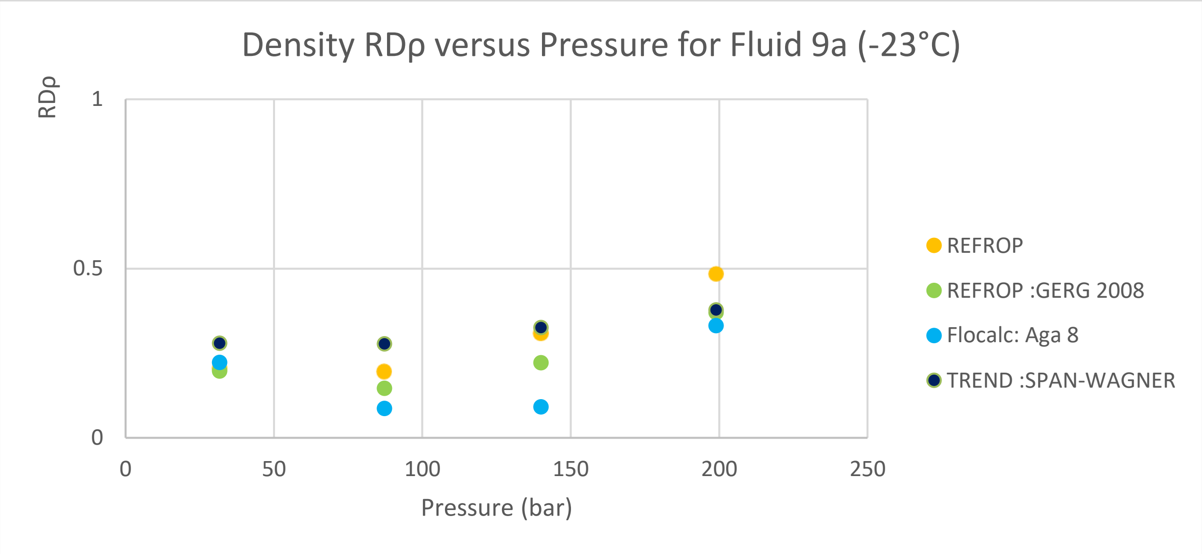

Figure 80: RDρ versus Pressure for Fluid 9a (-23°C)

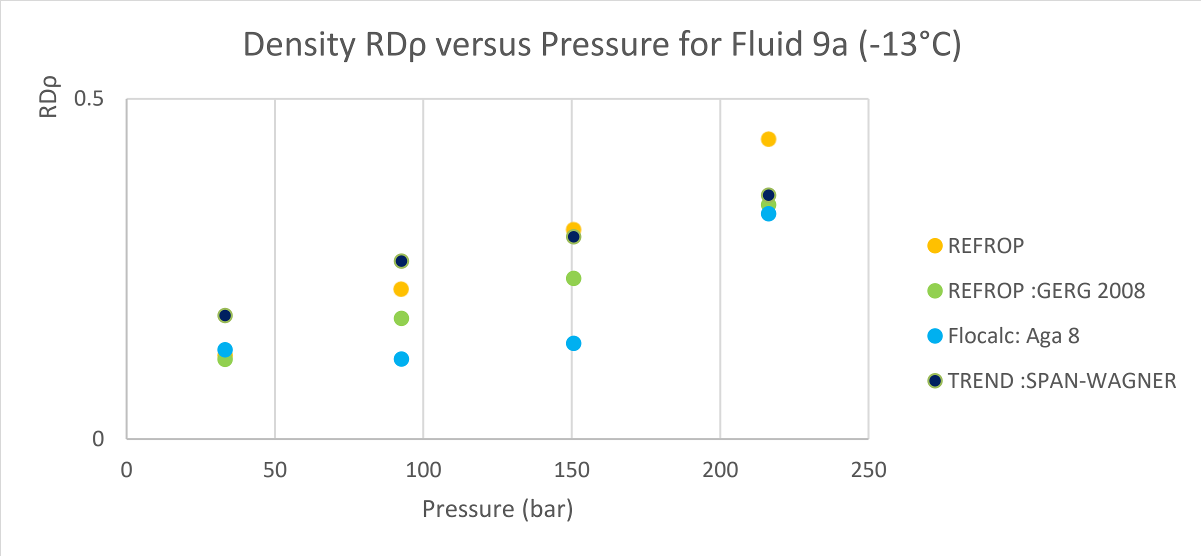

Figure 81: RDρ versus Pressure for Fluid 9a (-13°C)

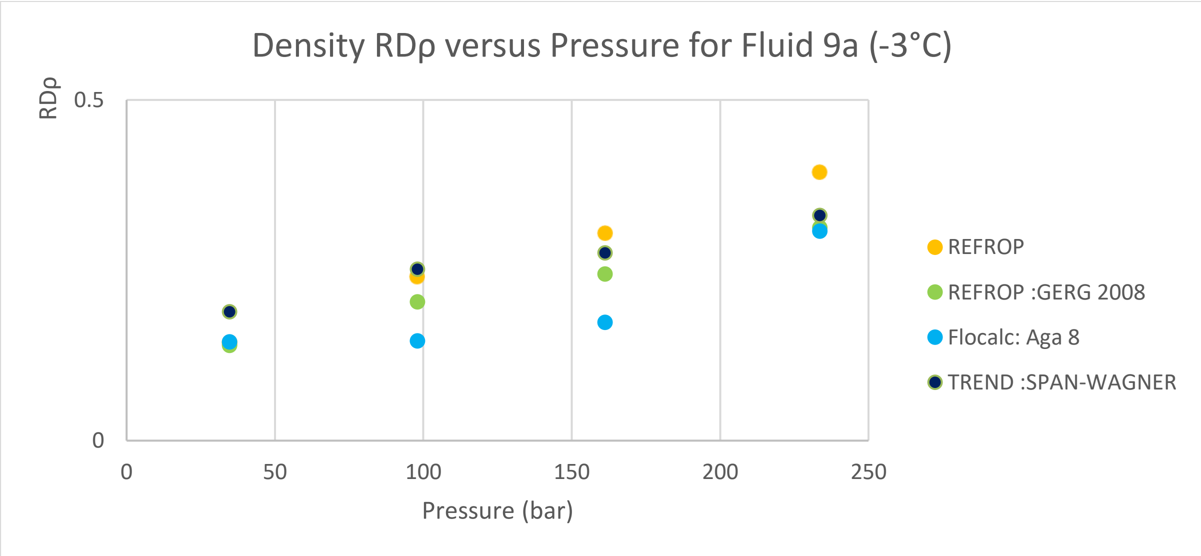

Figure 82: RDρ versus Pressure for Fluid 9a (-3°C)

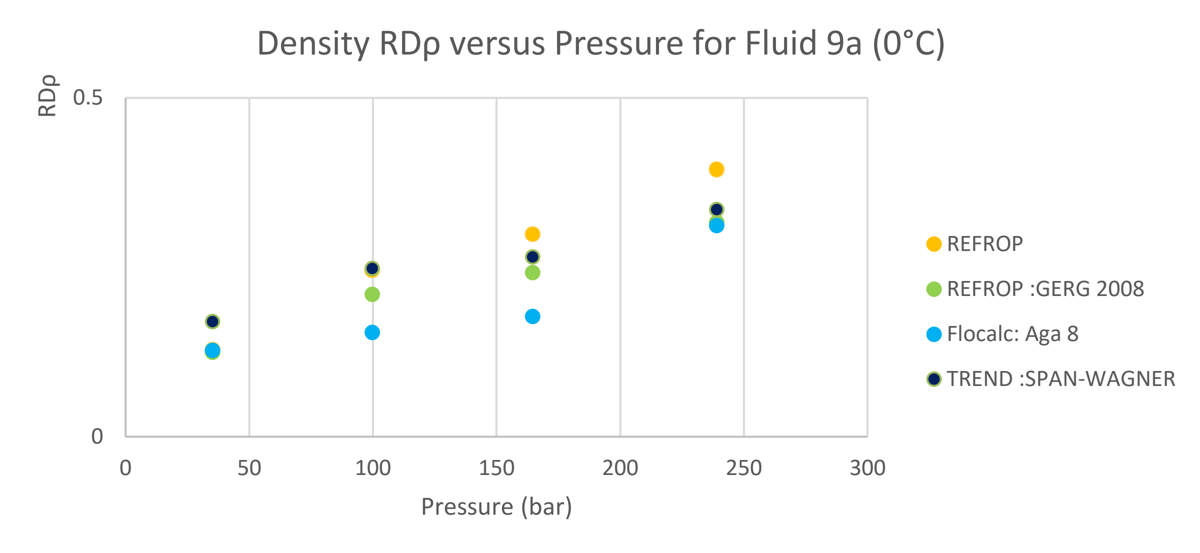

Figure 83: RDρ versus Pressure for Fluid 9a (0°C)

EoS	AADρ at (30 - 200 bar)				
	-33 °C	-23 °C	-13 °C	-3°C	0°C
REFPROP	0.317	0.298	0.273	0.271	0.267
GERG	0.240	0.234	0.219	0.225	0.223
Span - Wagner	0.355	0.315	0.275	0.261	0.255
AGA 8	**0.169**	**0.183**	**0.180**	**0.193**	**0.193**
PR	4.298	4.150	4.020	3.933	3.905
SRK	1.113	1.114	1.096	1.097	1.088
PC-SAFT	8.897	7.845	7.007	6.351	6.166

Table 37: Fluid 9a AADρ for each EoS

7.1.14 Fluid 9b(20% H_2 + 80% CH_4)

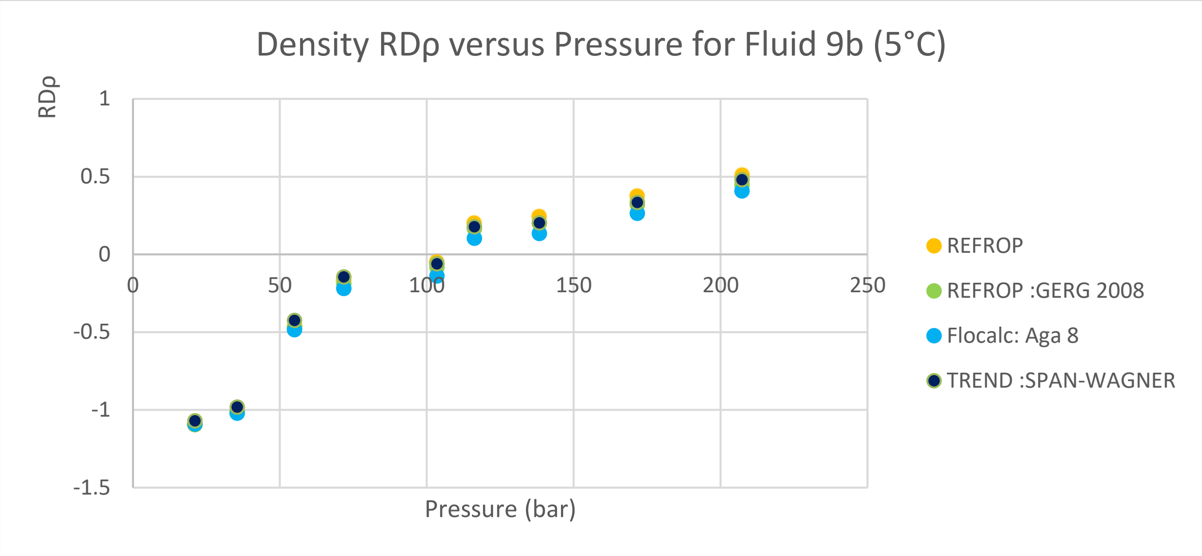

Figure 84: RDρ versus Pressure for Fluid 9b (5°C)

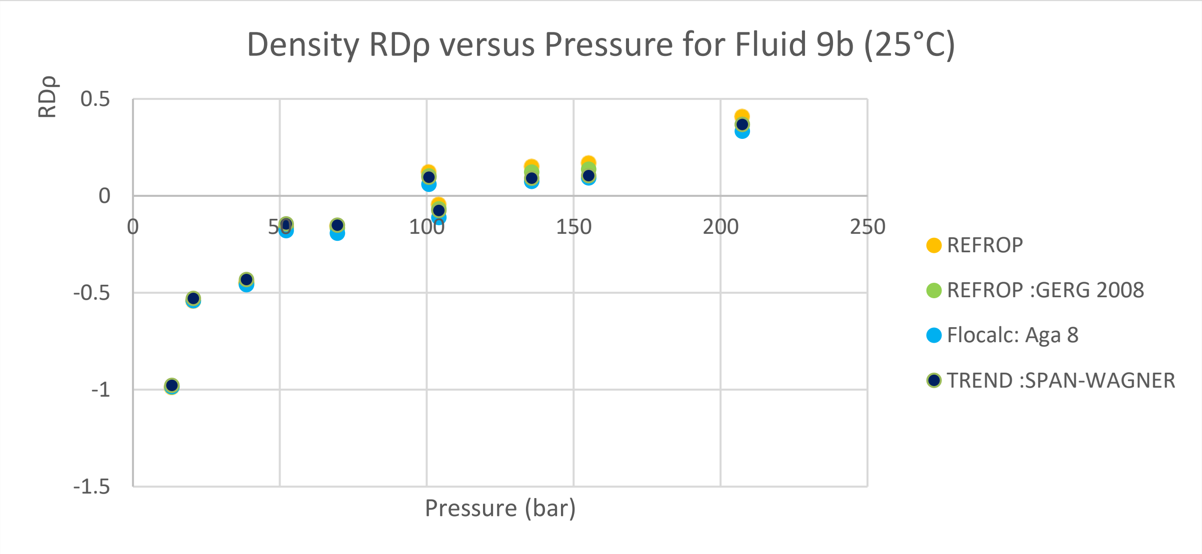

Figure 85: RDρ versus Pressure for Fluid 9b (25°C)

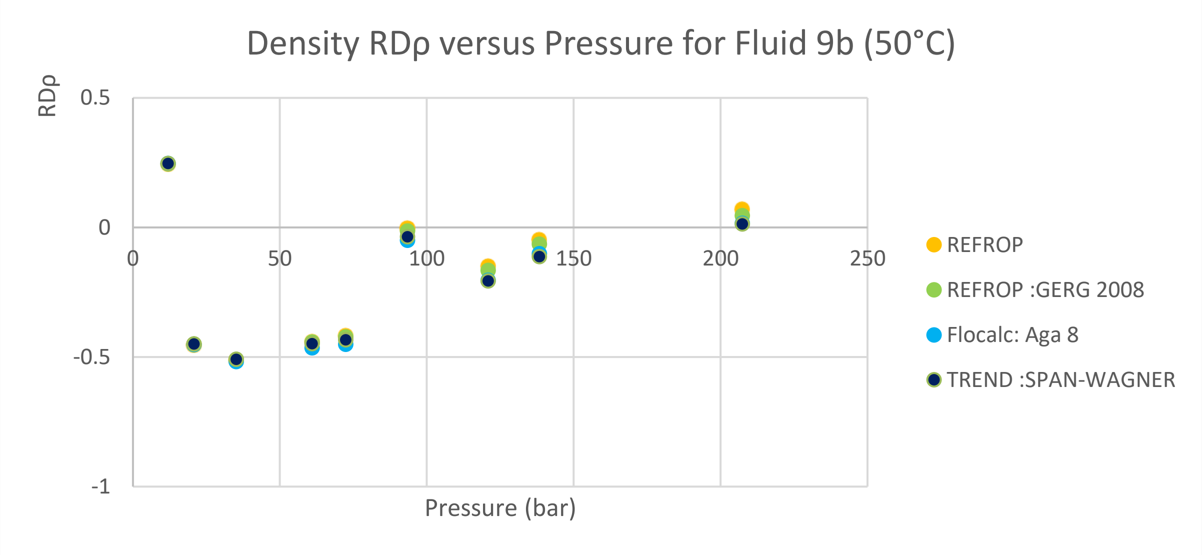

Figure 86: RDp versus Pressure for Fluid 9b (50°C)

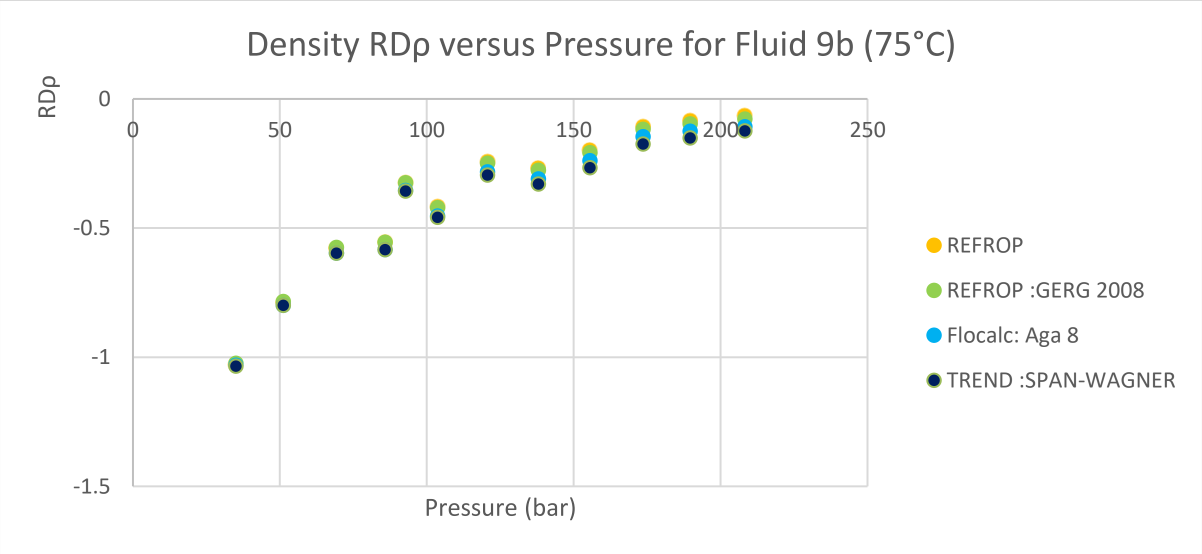

Figure 87: RDp versus Pressure for Fluid 9b (75°C)

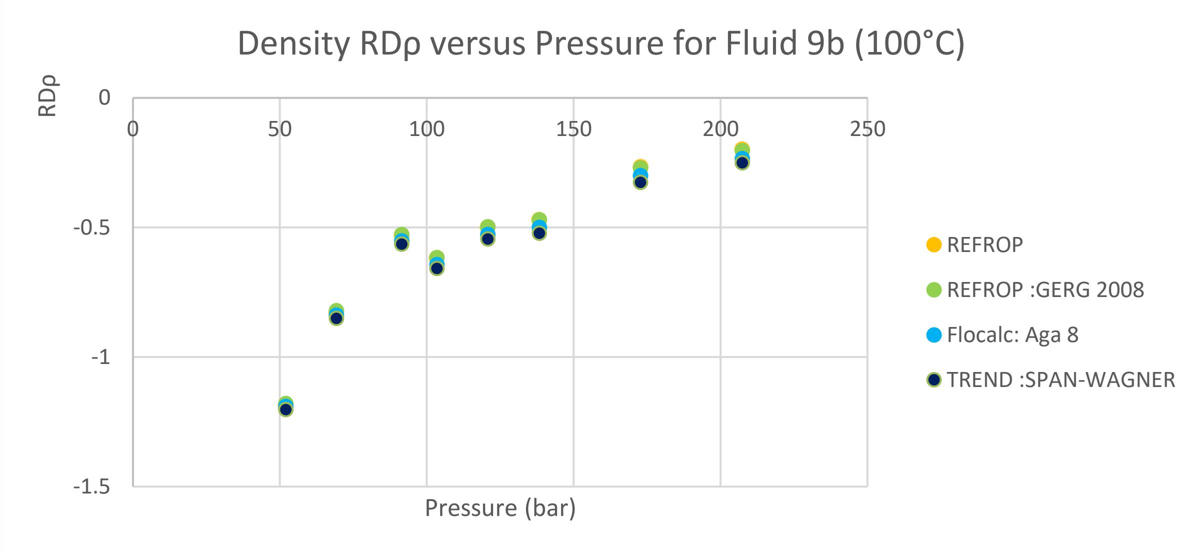

Figure 88: RDp versus Pressure for Fluid 9b (100°C)

EoS	AADp at (up to 200 bar)				
	5 °C	25 °C	50 °C	75°C	100°C
REFPROP	0.352	0.275	**0.260**	**0.389**	0.575
GERG	0.313	0.247	0.262	0.393	**0.573**
Span - Wagner	**0.263**	**0.215**	0.273	0.431	0.615
AGA 8	0.324	0.229	0.278	0.419	0.598
PR	4.743	4.046	2.093	2.274	1.878
SRK	1.428	1.154	0.775	1.165	1.313
PC-SAFT	5.039	3.994	2.498	2.599	1.912

Table 38: Fluid 9b AADp for each EoS

7.2 Speed of sound

Fluid	H2	CH4	C2H6	C3H8	iC4	nC4	iC5	nC5	neoC5	C6	N2	Co2	He
1	0.03	0.7885	0.0075	0.003	0.002	0.002	0.0005	0.0005	0.0005	0.0005	0.12	0.04	0.005
2	0.05	0.836	0.057	0.019	0.0019	0.00285					0.01425	0.019	
3	0.1	0.792	0.054	0.018	0.0018	0.0027					0.0135	0.018	
4	0.15	0.748	0.051	0.017	0.0017	0.00255					0.01275	0.017	
5	0.20	0.704	0.048	0.016	0.0016	0.0024					0.012	0.016	
6	0.05	0.95											
7	0.10	0.90											

Table 39: Composition used for NG with up to 20% hydrogen mixtures SoS calculations

7.2.1 Fluid 1 (3% H_2 + NG)

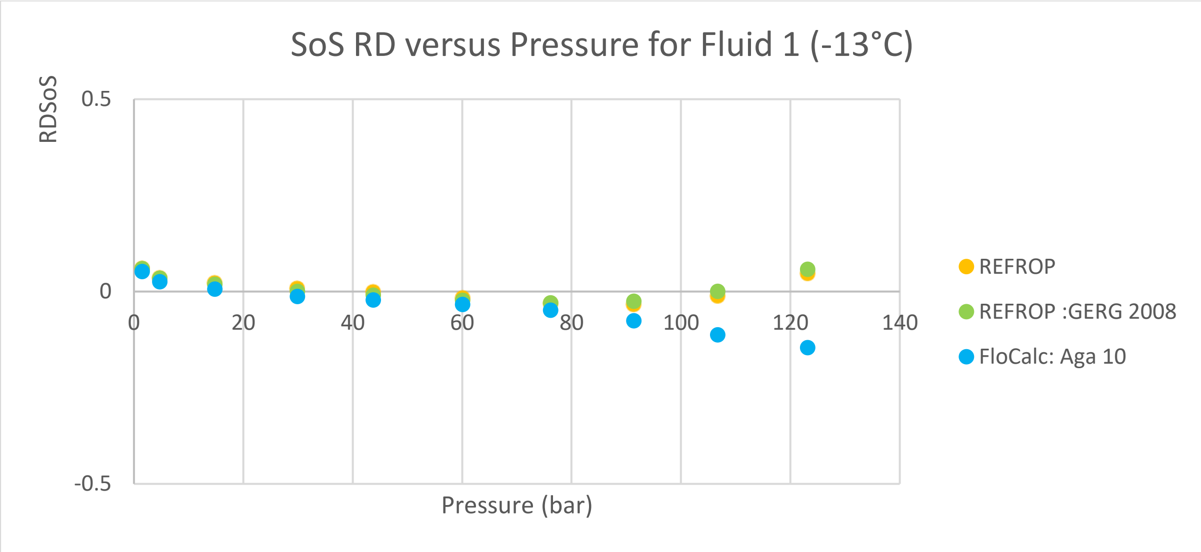

Figure 89: RD SoS versus Pressure for Fluid 1 (-13°C)

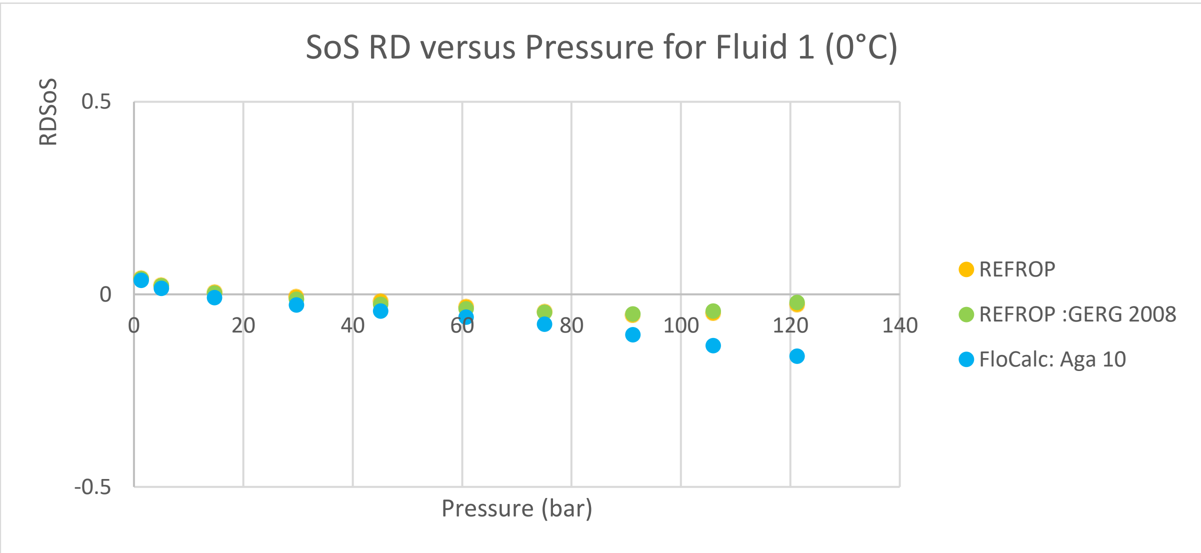

Figure 90: RD SoS versus Pressure for Fluid 1 (0°C)

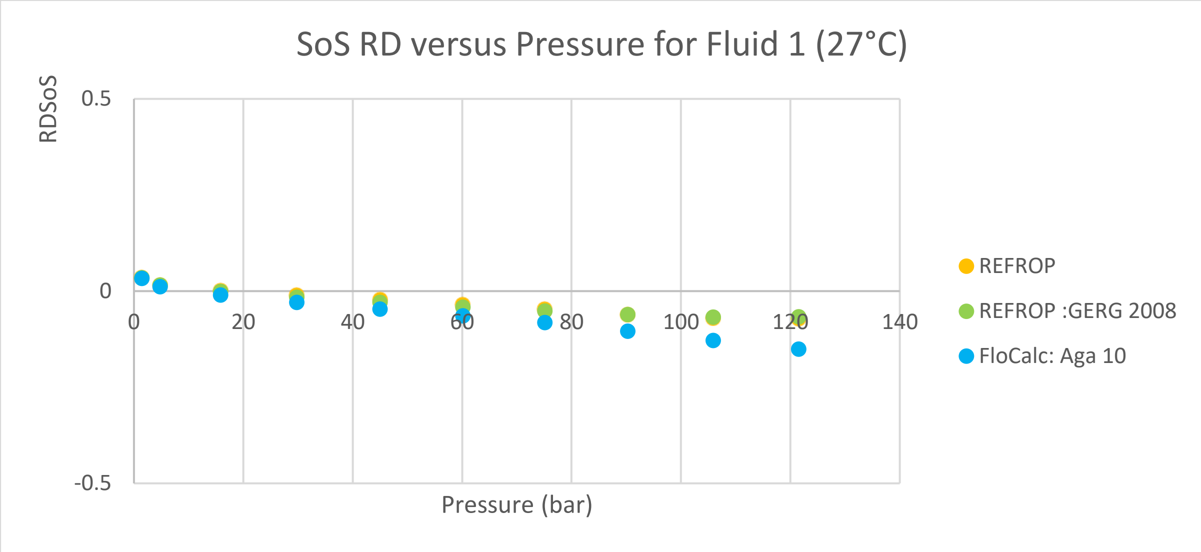

Figure 91: RD SoS versus Pressure for Fluid 1 (27°C)

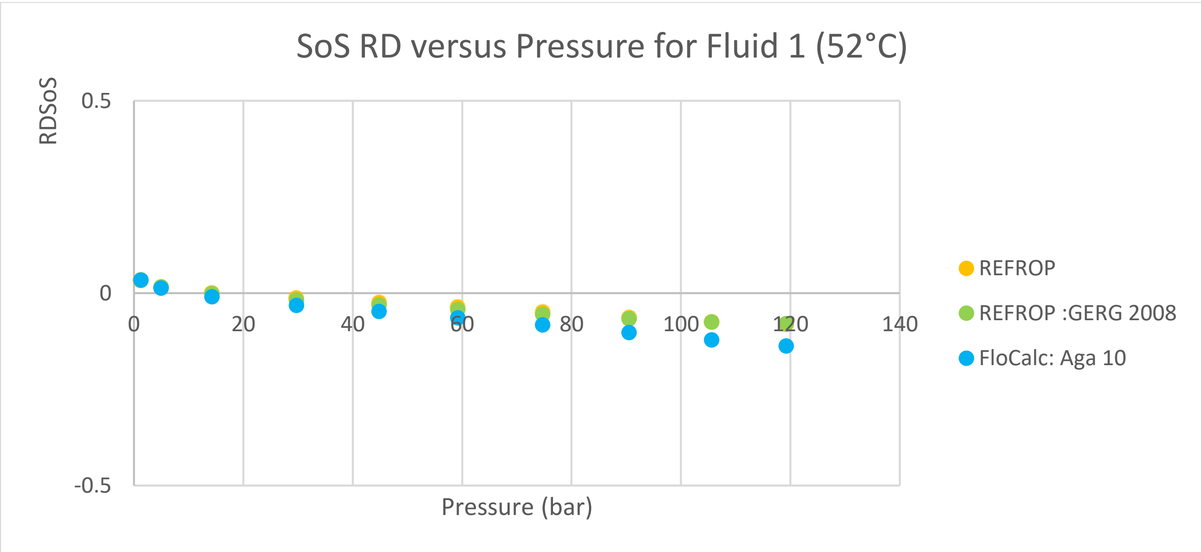

Figure 92: RD SoS versus Pressure for Fluid 1 (52°C)

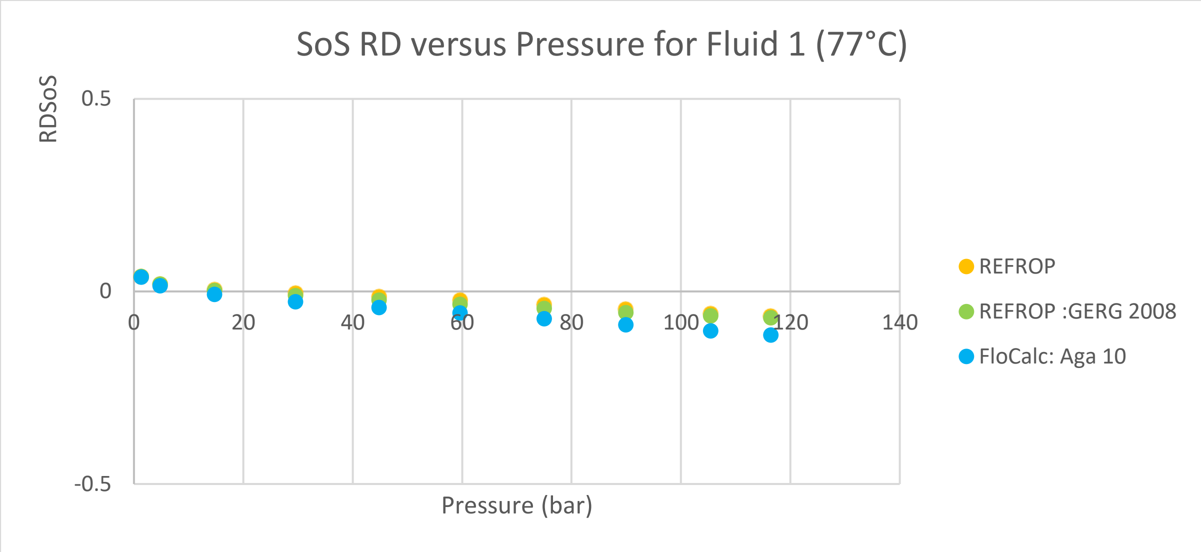

Figure 93: RD SoS versus Pressure for Fluid 1 (77°C)

EoS	AAD SoS at (1 up to 120 bar)				
	-13 °C	0°C	27°C	52°C	77 °C
REFPROP	0.027	0.030	**0.037**	**0.039**	**0.031**
GERG	**0.026**	0.030	0.039	0.042	0.036
AGA 10	0.054	0.067	0.066	0.064	0.056

Table 40: Fluid 1 AAD Sos for each EoS

7.2.2 Fluid 2 (5% H_2 + NG)

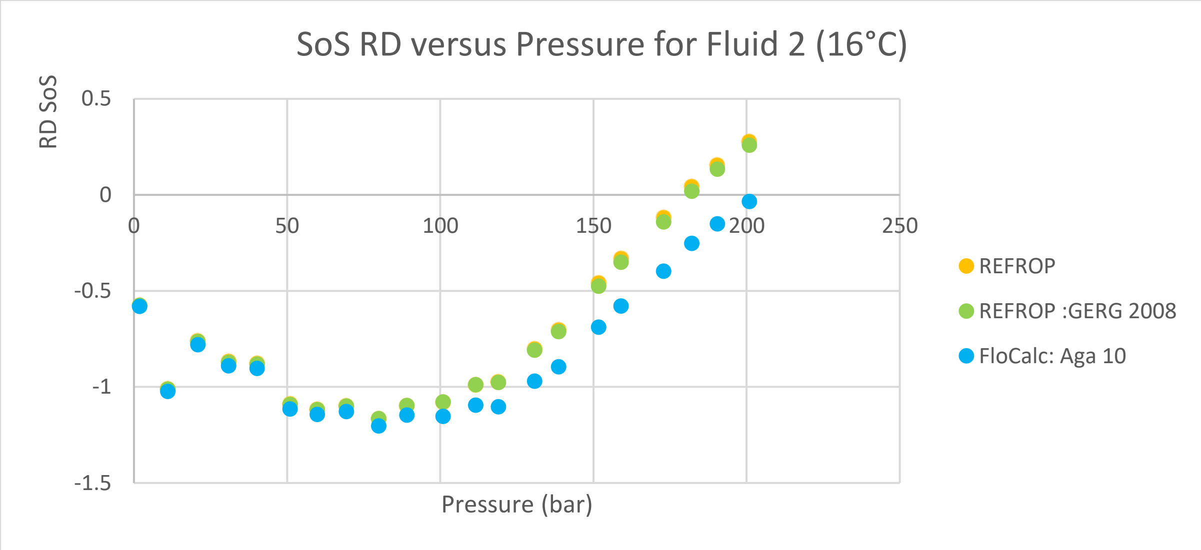

Figure 94: RD SoS versus Pressure for Fluid 2 (16°C)

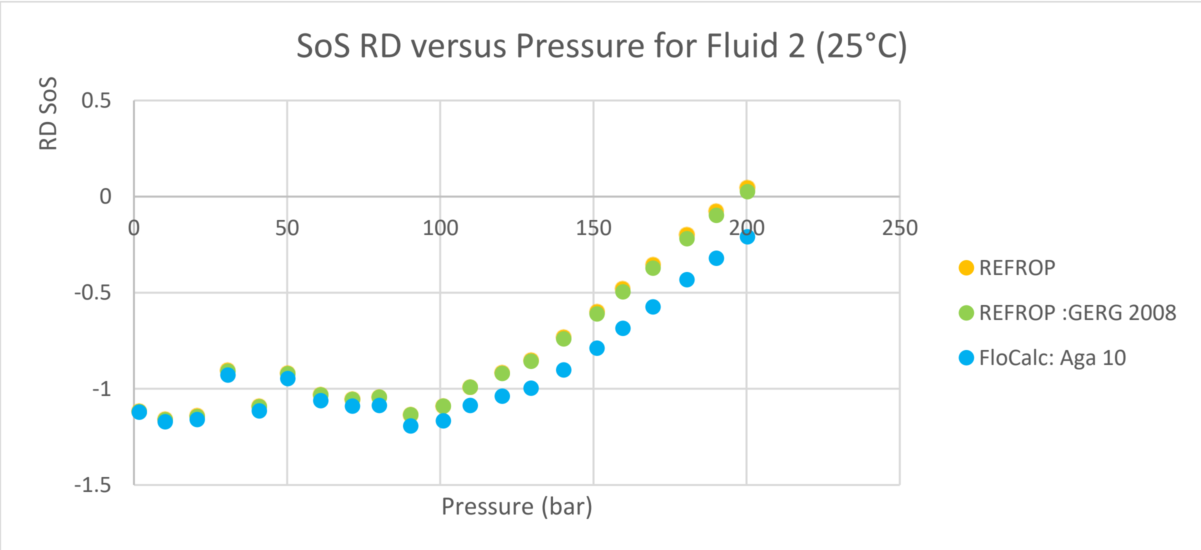

Figure 95: RD SoS versus Pressure for Fluid 2 (25°C)

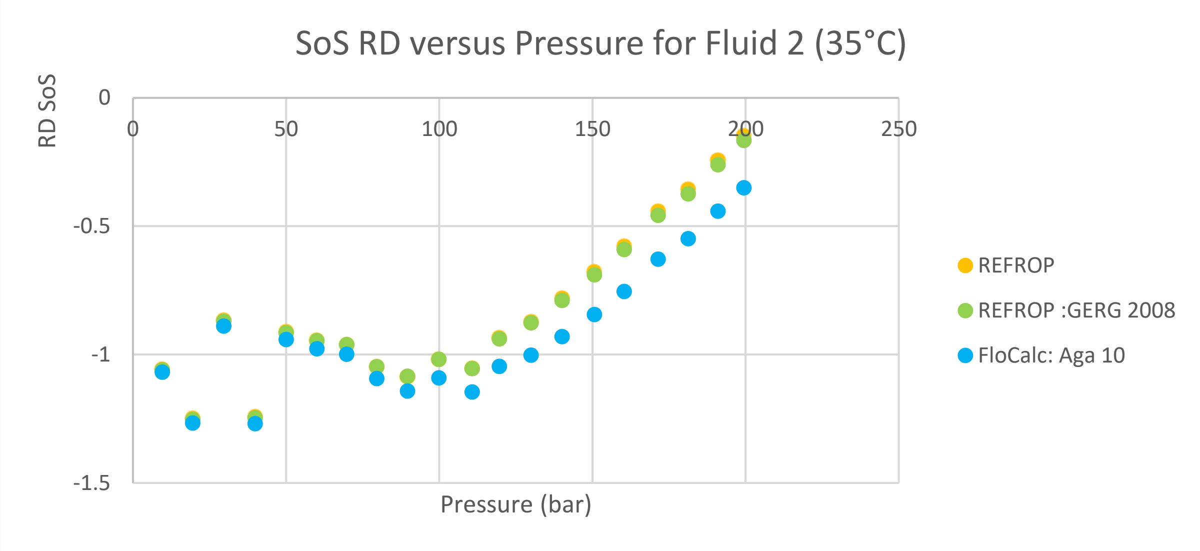

Figure 96: RD SoS versus Pressure for Fluid 2 (35°C)

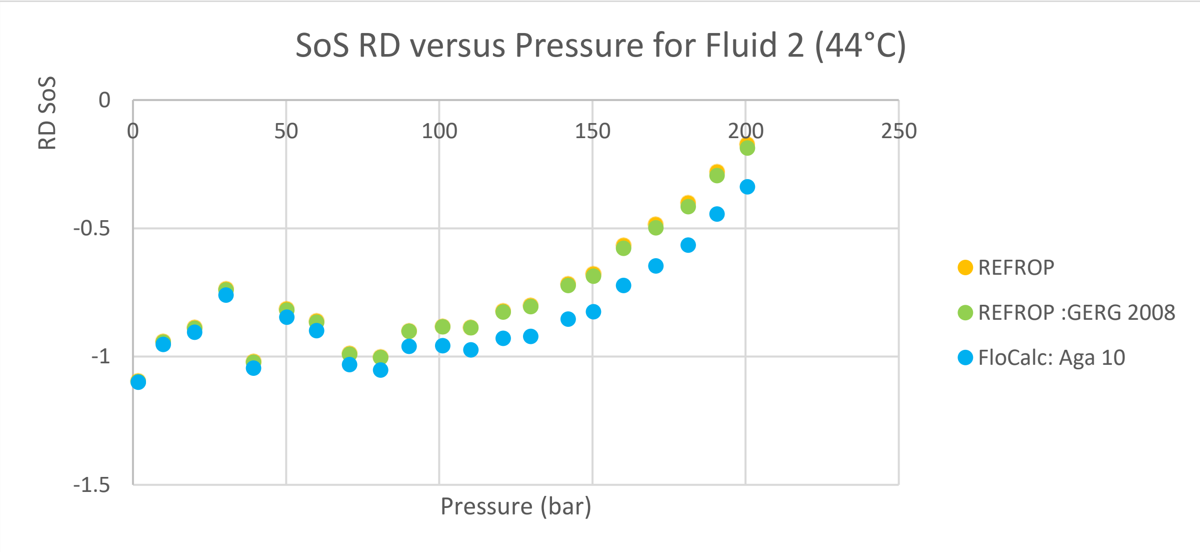

Figure 97: RD SoS versus Pressure for Fluid 2 (44°C)

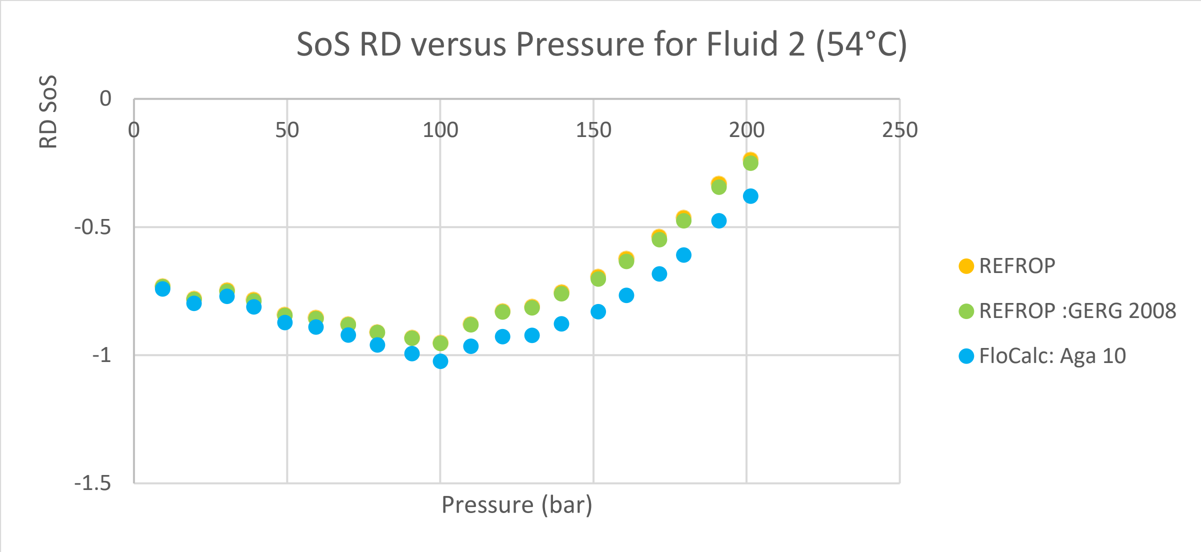

Figure 98: RD SoS versus Pressure for Fluid 2 (54°C)

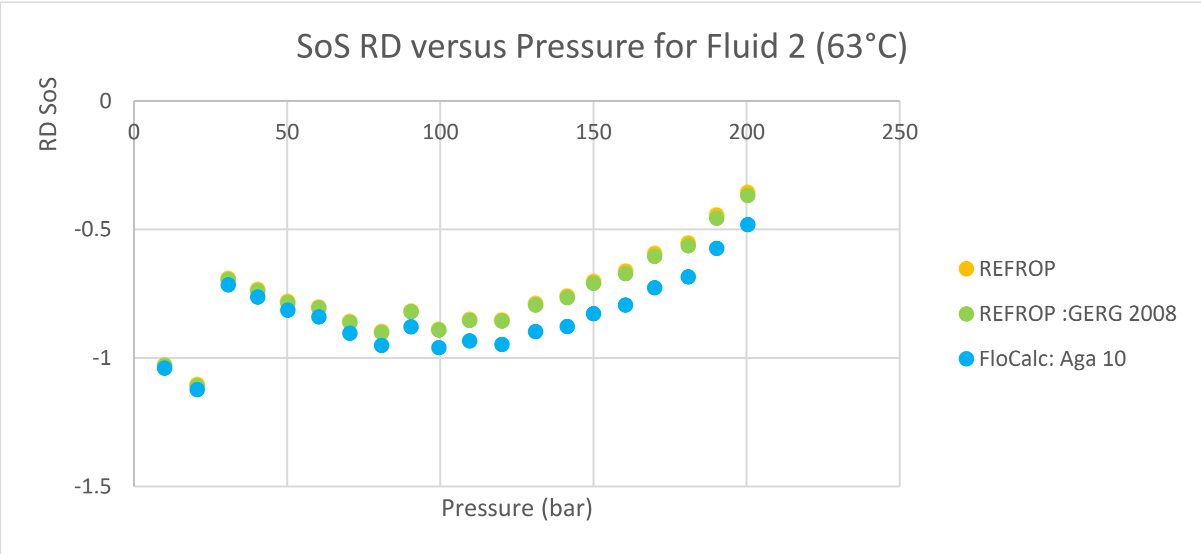

Figure 99: RD SoS versus Pressure for Fluid 2 (63°C)

EoS	AAD SoS at (1 up to 120 bar)					
	16 °C	25°C	35°C	44°C	54 °C	63 °C
REFPROP	**1.010**	**1.039**	**1.030**	**0.895**	**0.843**	**0.859**
GERG	1.012	1.041	1.032	0.898	0.846	0.862
AGA 10	1.057	1.086	1.077	0.942	0.890	0.906

Table 41: Fluid 2 AAD SoS for each EoS over pressure range of up to 120 bar

EoS	AAD SoS at (1 up to 200 bar)					
	16 °C	25°C	35°C	44°C	54 °C	63 °C
REFPROP	**0.742**	**0.806**	**0.823**	**0.759**	**0.728**	**0.758**
GERG	0.743	0.811	0.830	0.765	0.734	0.764
AGA 10	0.820	0.908	0.921	0.844	0.811	0.836

Table 42: Fluid 2 AAD SoS for each EoS over pressure range of up to 200 bar

7.2.3 **Fluid 3 (10% H_2 + NG)**

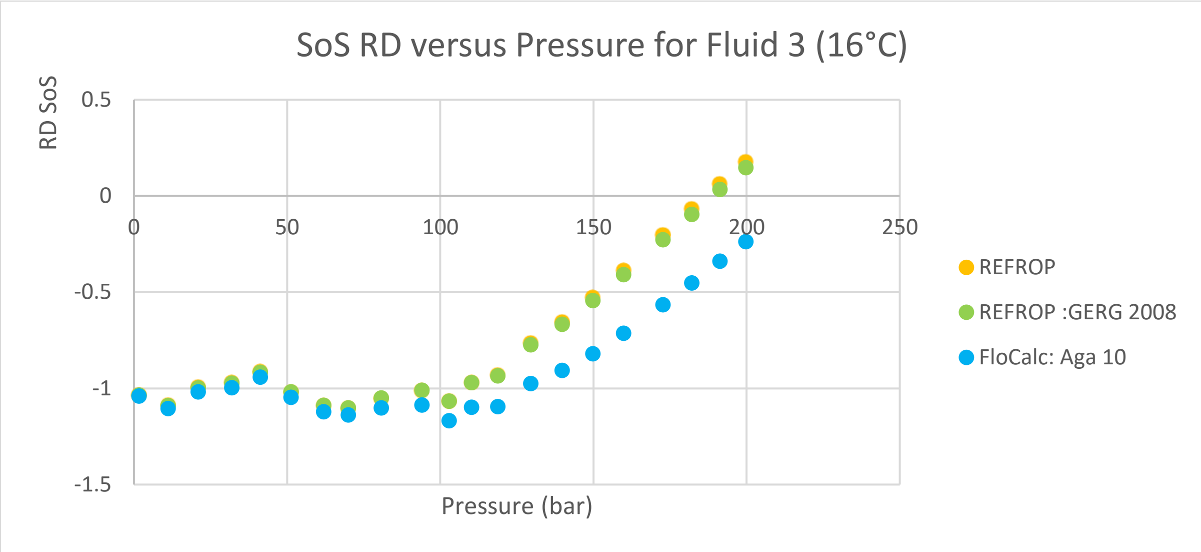

Figure 100: RD SoS versus Pressure for Fluid 3 (16°C)

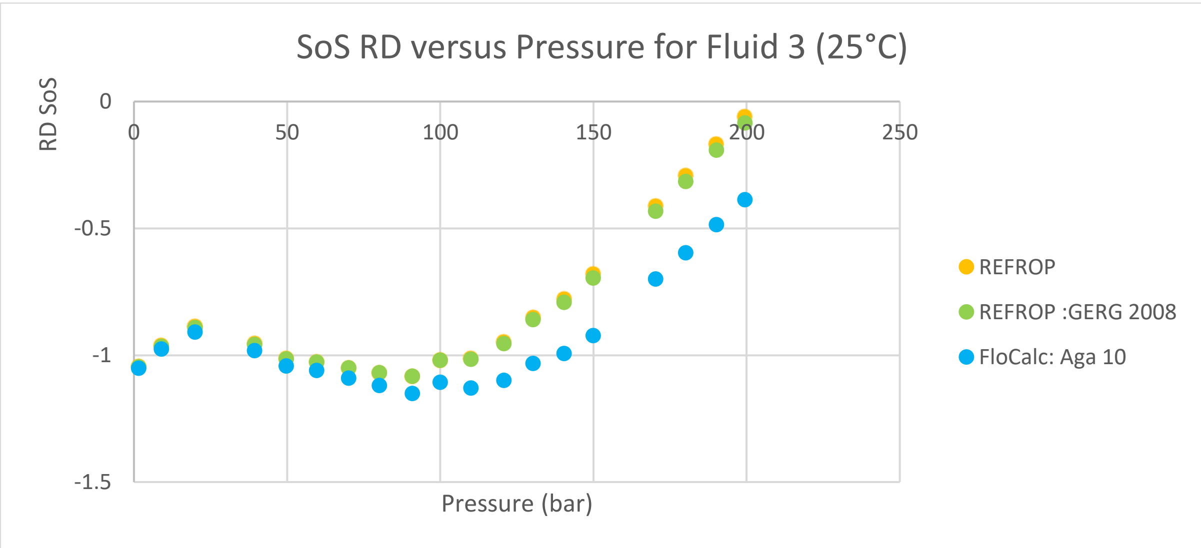

Figure 101: RD SoS versus Pressure for Fluid 3 (25°C)

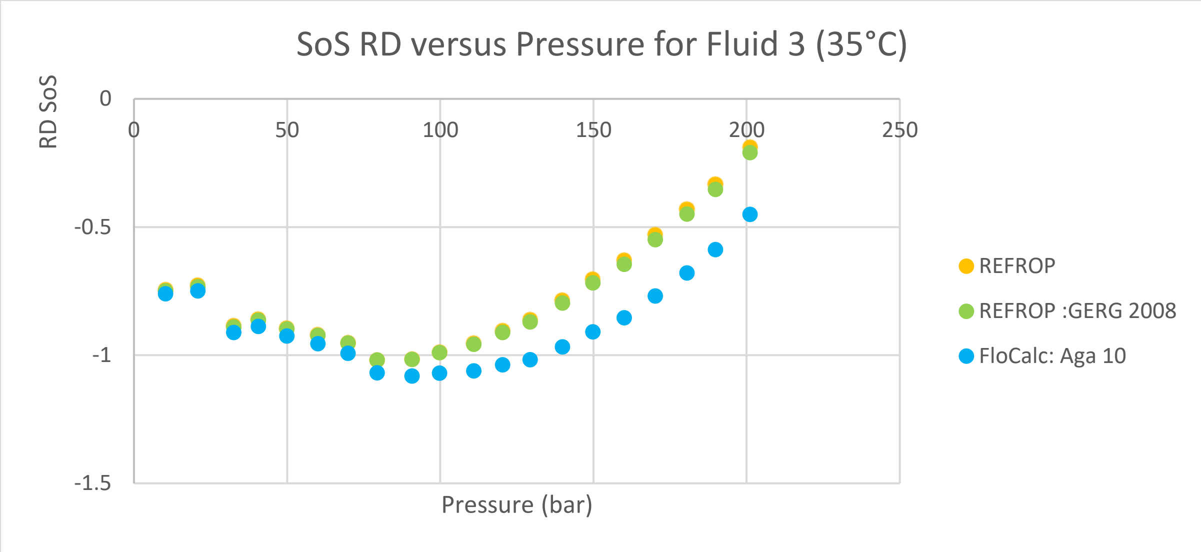

Figure 102: RD SoS versus Pressure for Fluid 3 (35°C)

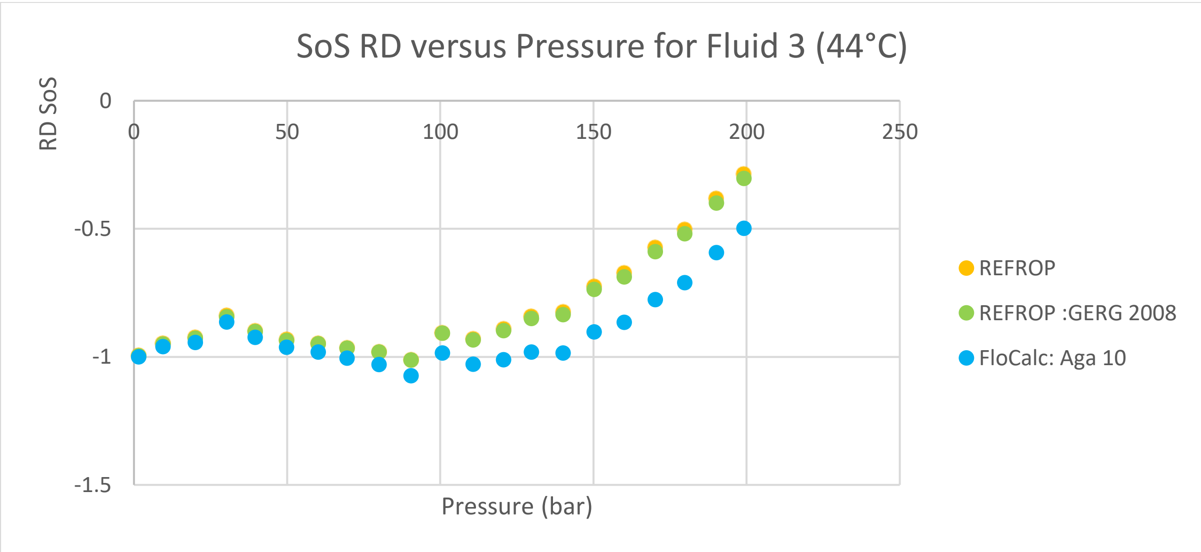

Figure 103: RD SoS versus Pressure for Fluid 3 (44°C)

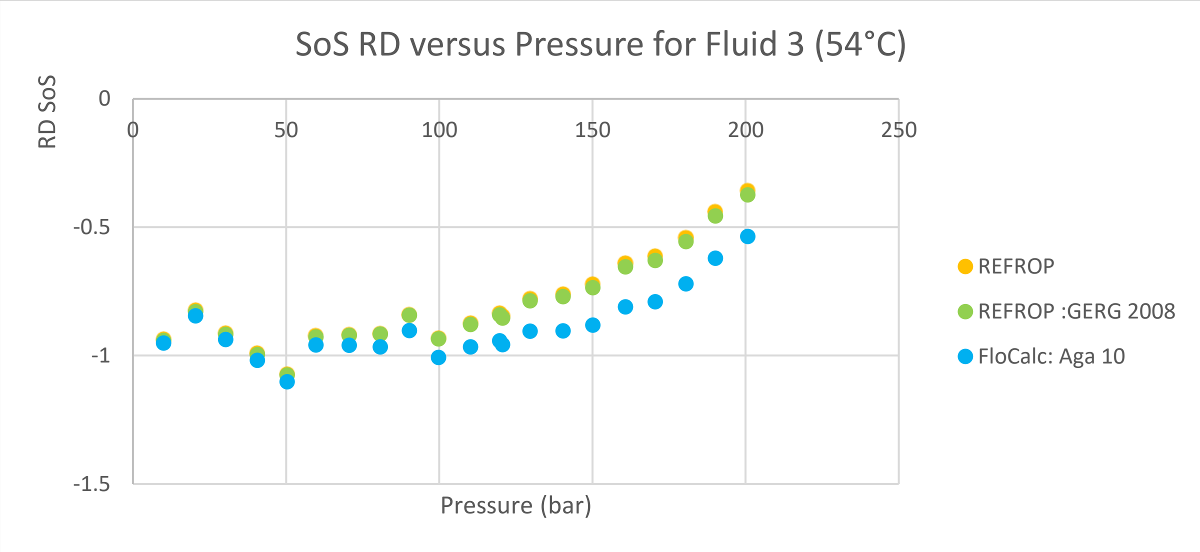

Figure 104: RD SoS versus Pressure for Fluid 3 (54°C)

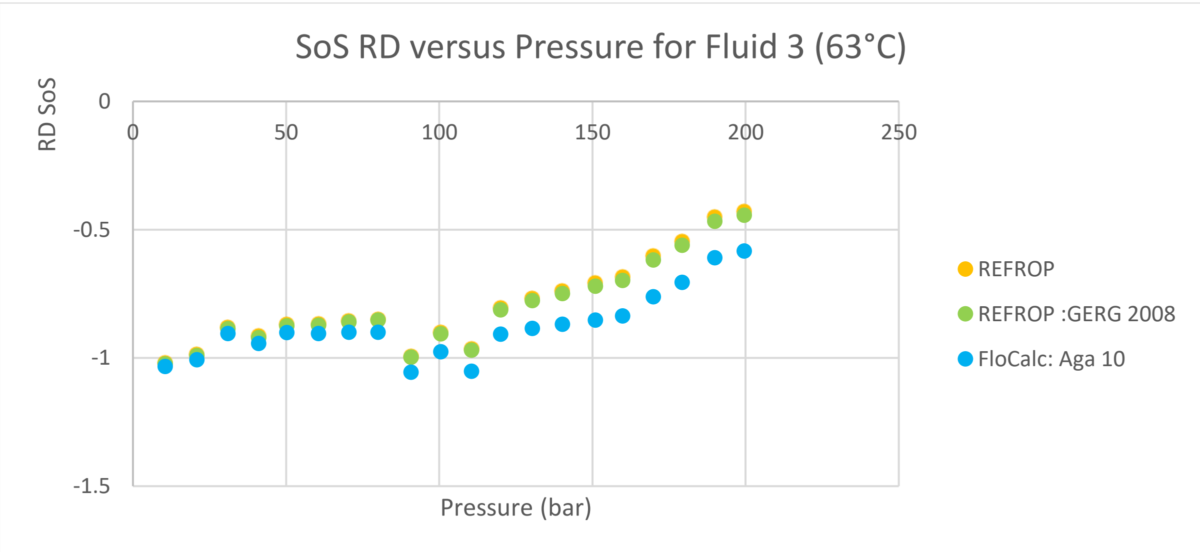

Figure 105: RD SoS versus Pressure for Fluid 3 (63°C) 5

EoS	AAD SoS at (1 up to 200 bar)					
	16 °C	25°C	35°C	44°C	54 °C	63 °C
REFPROP	**0.766**	**0.806**	**0.767**	**0.809**	**0.794**	**0.792**
GERG	0.770	0.814	0.775	0.816	0.802	0.800
AGA 10	0.904	0.938	0.887	0.909	0.889	0.880

Table 43: Fluid 3 AAD SoS for each EoS

7.2.4 Fluid 4 (15% H_2 + NG)

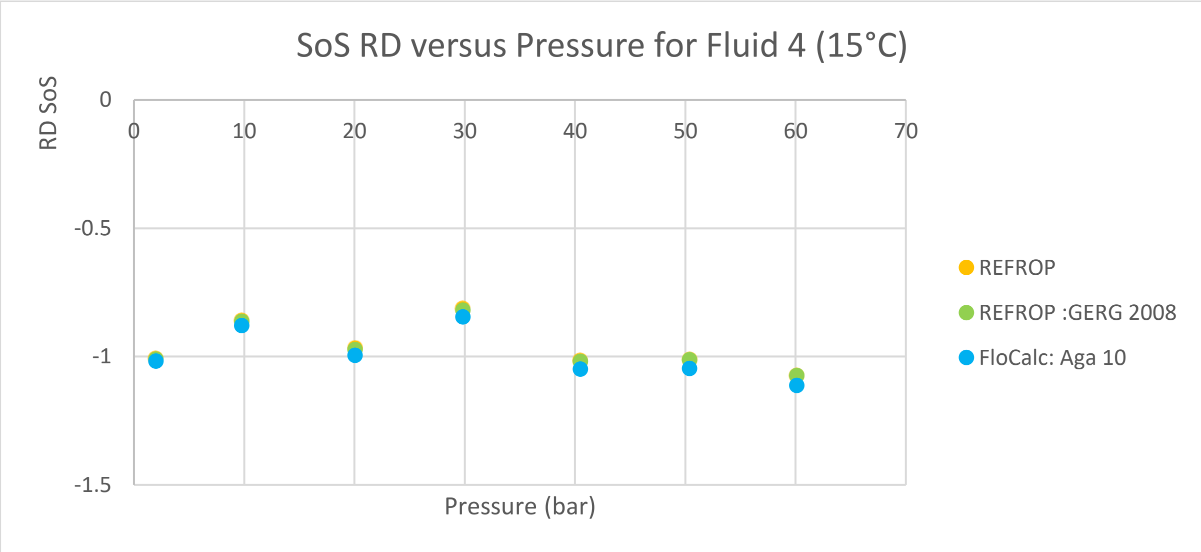

Figure 106: RD SoS versus Pressure for Fluid 4 (15°C) 6

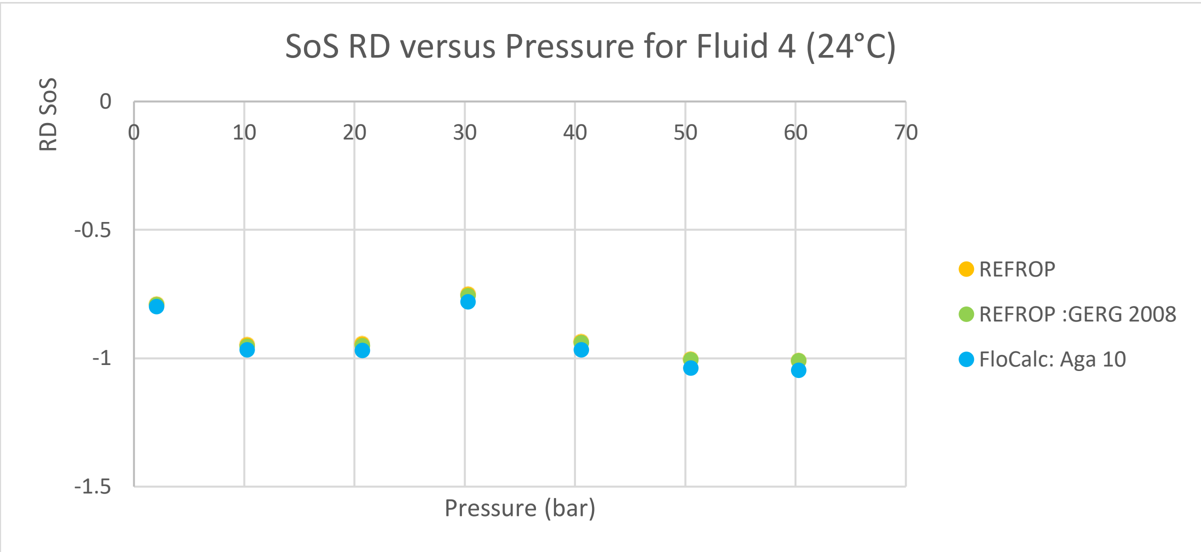

Figure 107: RD SoS versus Pressure for Fluid 4 (24°C) 7

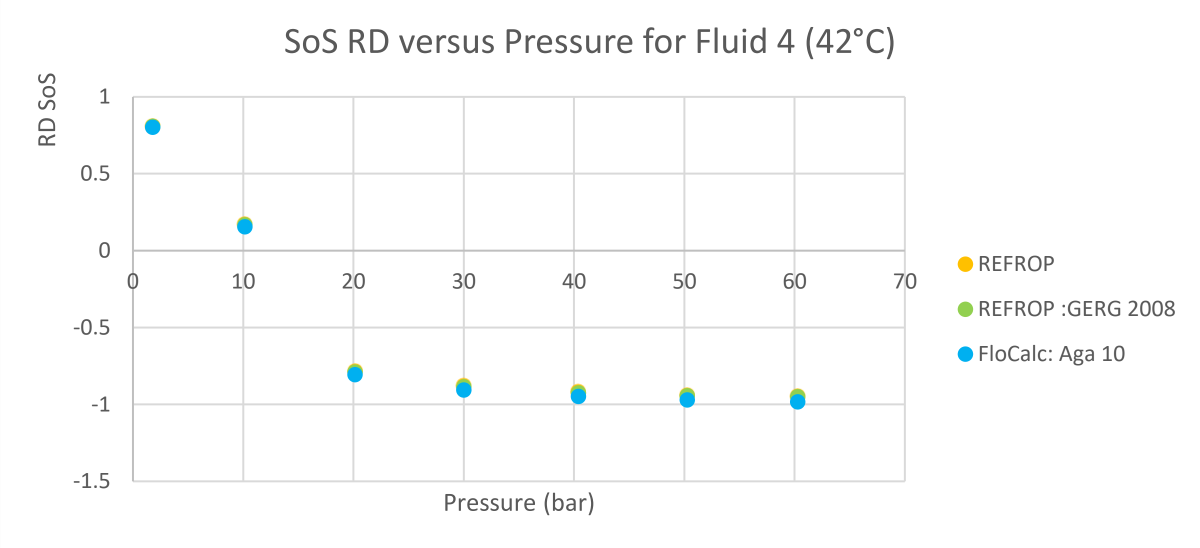

Figure 108: RD SoS versus Pressure for Fluid 4 (42°C) 8

EoS	AAD SoS at (1 up to 60 bar)		
	15 °C	24 °C	42.5 °C
REFPROP	**0.964**	**0.912**	**0.778**
GERG	0.967	0.915	0.781
AGA 10	0.992	0.938	0.796

Table 44: Fluid 4 AAD SoS for each EoS

7.2.5 Fluid 5 (20% H_2 + NG)

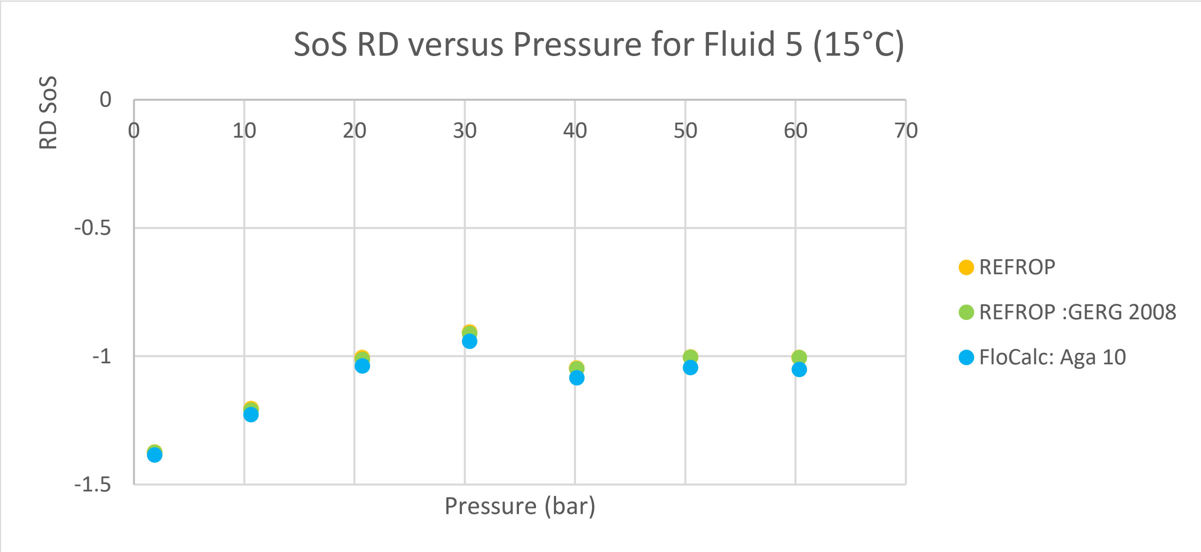

Figure 109: RD SoS versus Pressure for Fluid 5 (15°C)

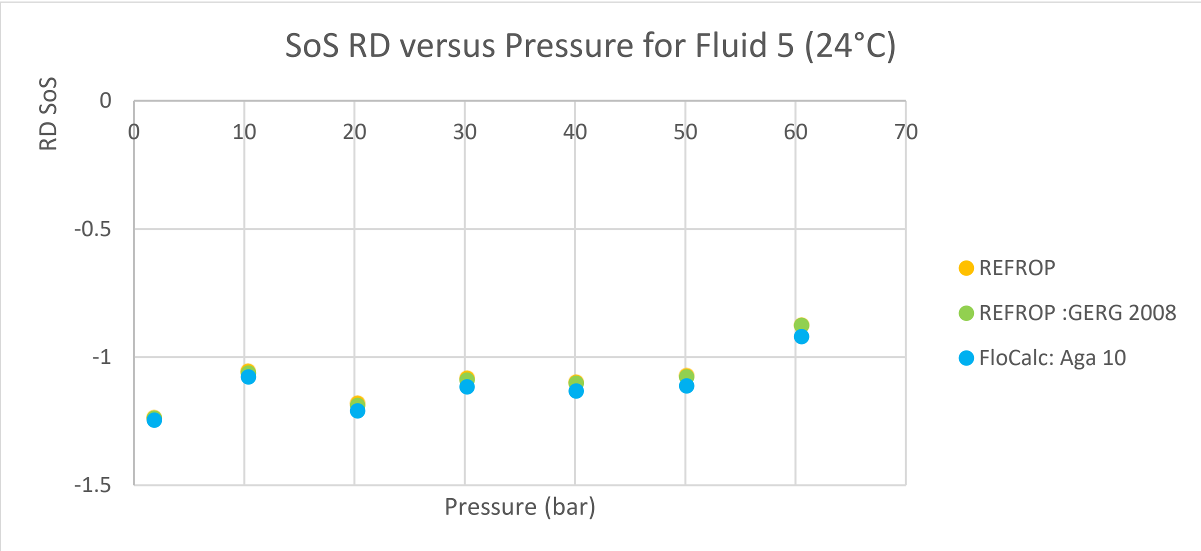

Figure 110: RD SoS versus Pressure for Fluid 5 (24°C)

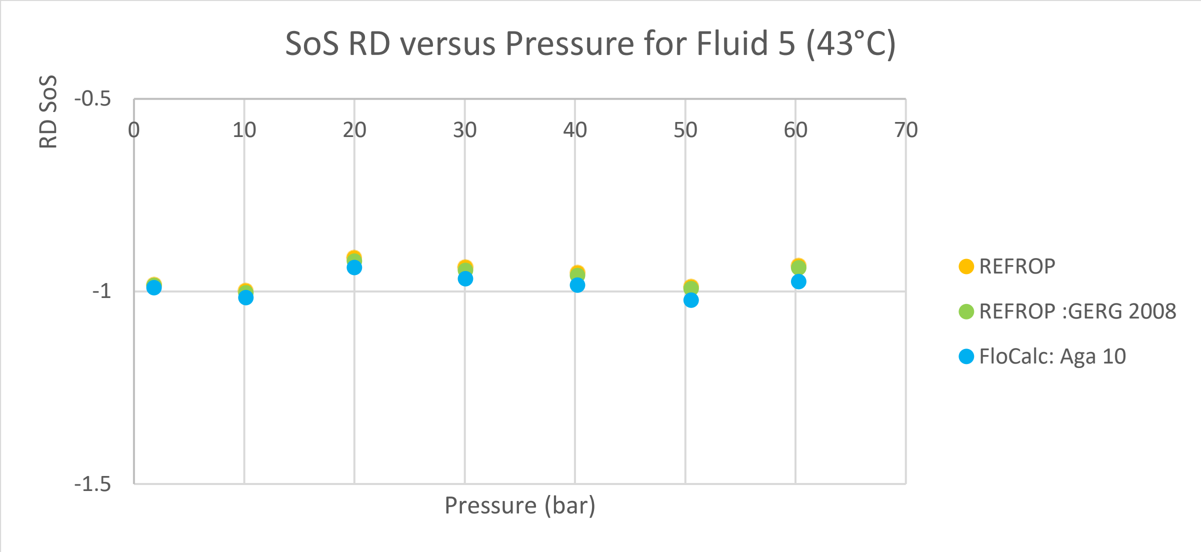

Figure 111: RD SoS versus Pressure for Fluid 5 (43°C)

EoS	AAD SoS at (1 up to 60 bar)		
	15 °C	24 °C	42.5 °C
REFPROP	**1.077**	**1.086**	**0.958**
GERG	1.082	1.091	0.964
AGA 10	1.111	1.116	0.984

Table 45: Fluid 5 AAD SoS for each EoS

7.2.6 Fluid 6 (5% H_2 + 95% CH_4)

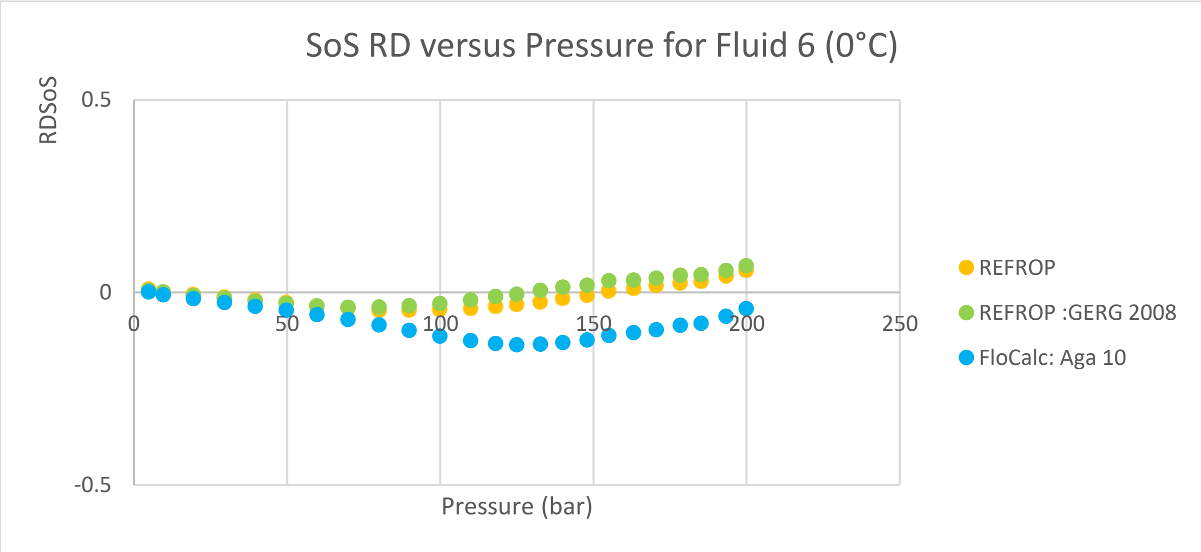

Figure 112: RD SoS versus Pressure for Fluid 6 (0°C)

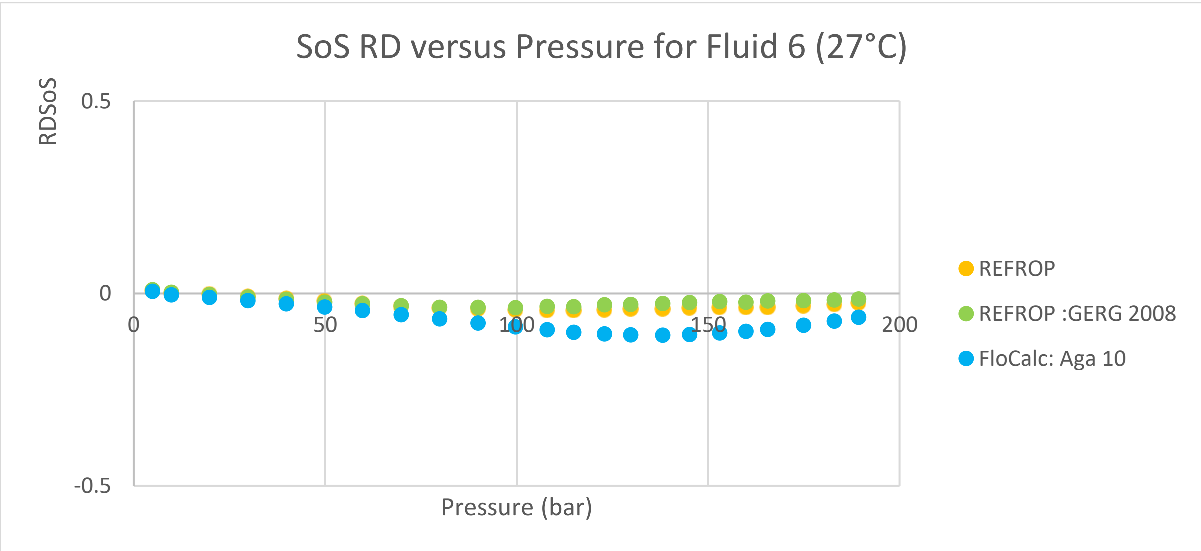

Figure 113: RD SoS versus Pressure for Fluid 6 (27°C)

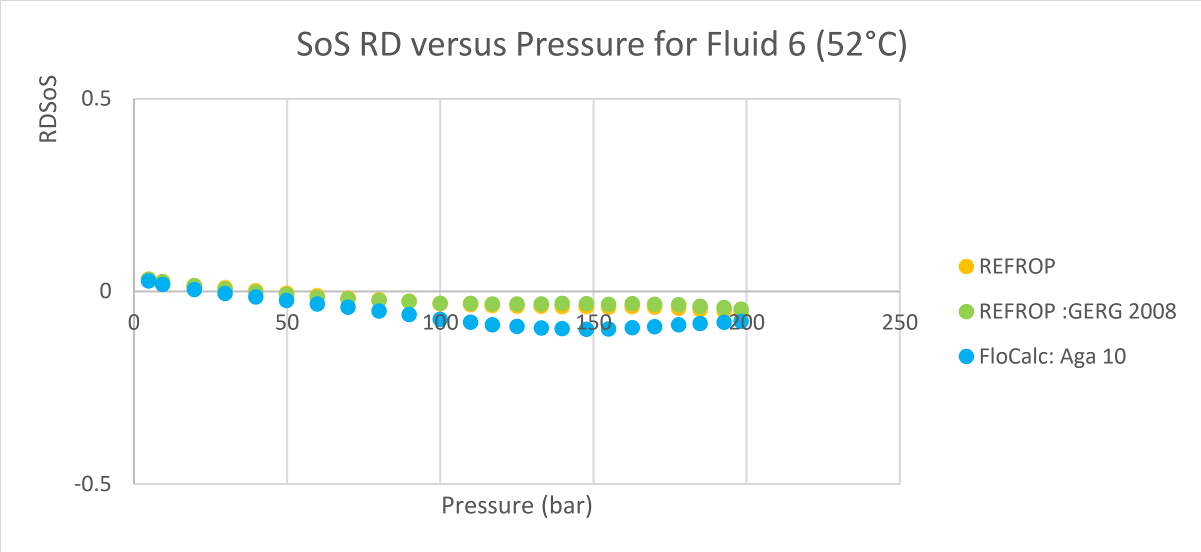

Figure 114: RD SoS versus Pressure for Fluid 6 (52°C)

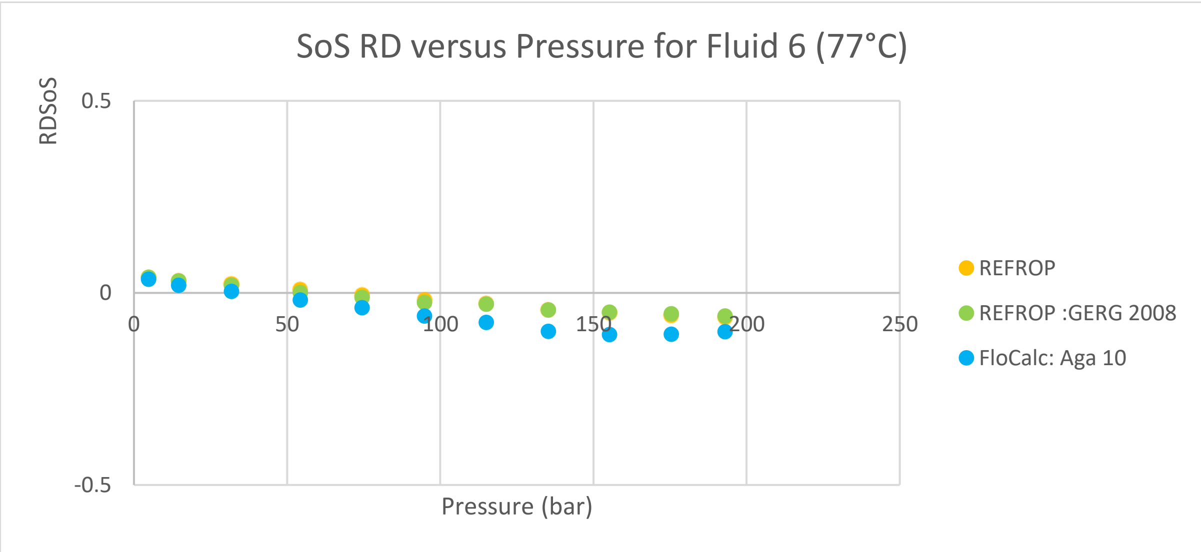

Figure 115: RD SoS versus Pressure for Fluid 6 (77°C)

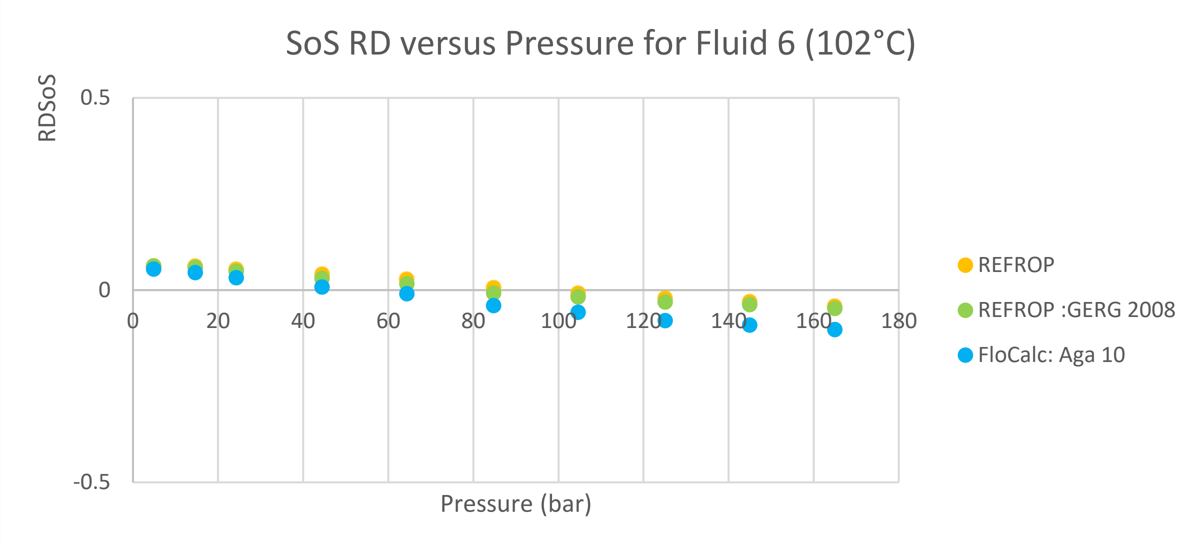

Figure 116: RD SoS versus Pressure for Fluid 6 (102°C)

EoS	AAD SoS at (5 up to 200 bar)				
	0 °C	27°C	52°C	77°C	102 °C
REFPROP	**0.026**	0.029	0.031	0.034	**0.035**
GERG	0.027	**0.022**	**0.027**	**0.033**	0.036
AGA 10	0.080	0.068	0.063	0.061	0.052

Table 46: Fluid 6 AAD SoS for each EoS

7.2.7 Fluid 7 (10% H_2 + 90% CH_4)

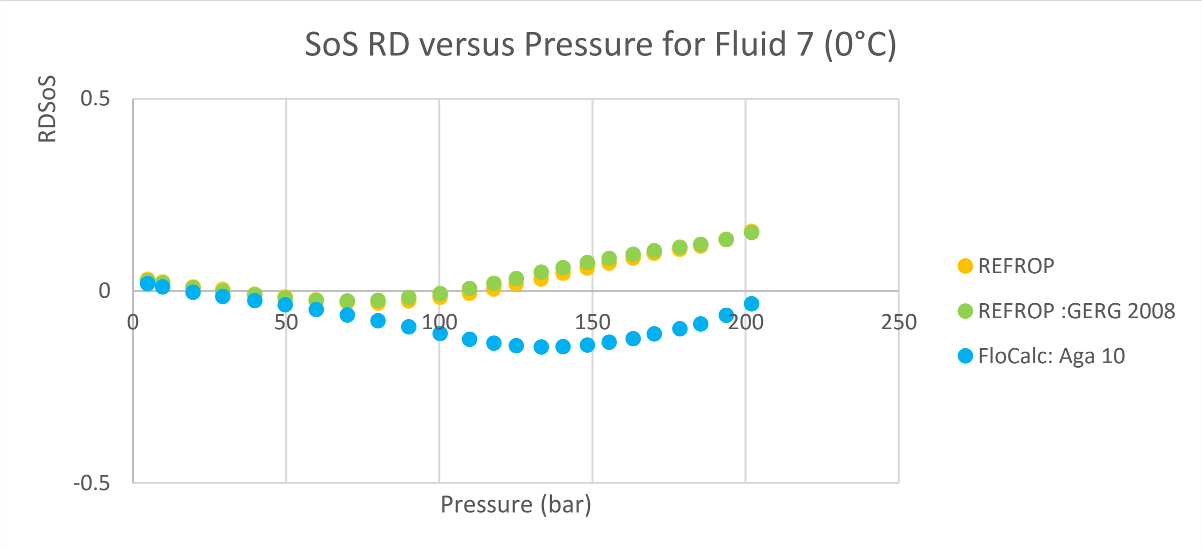

Figure 117: RD SoS versus Pressure for Fluid 7 (0°C)

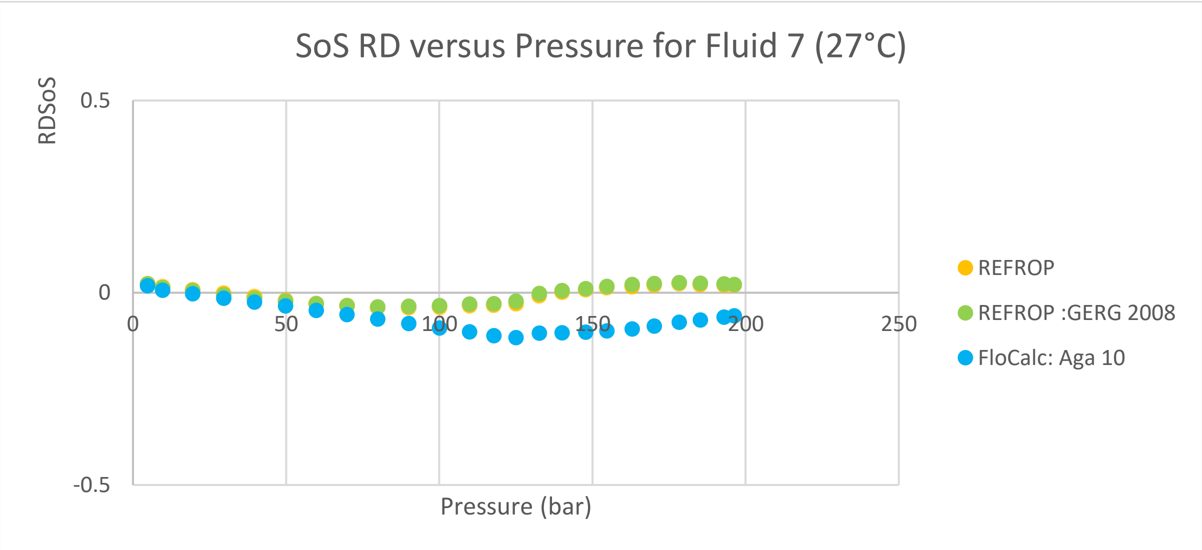

Figure 118: RD SoS versus Pressure for Fluid 7 (27°C)

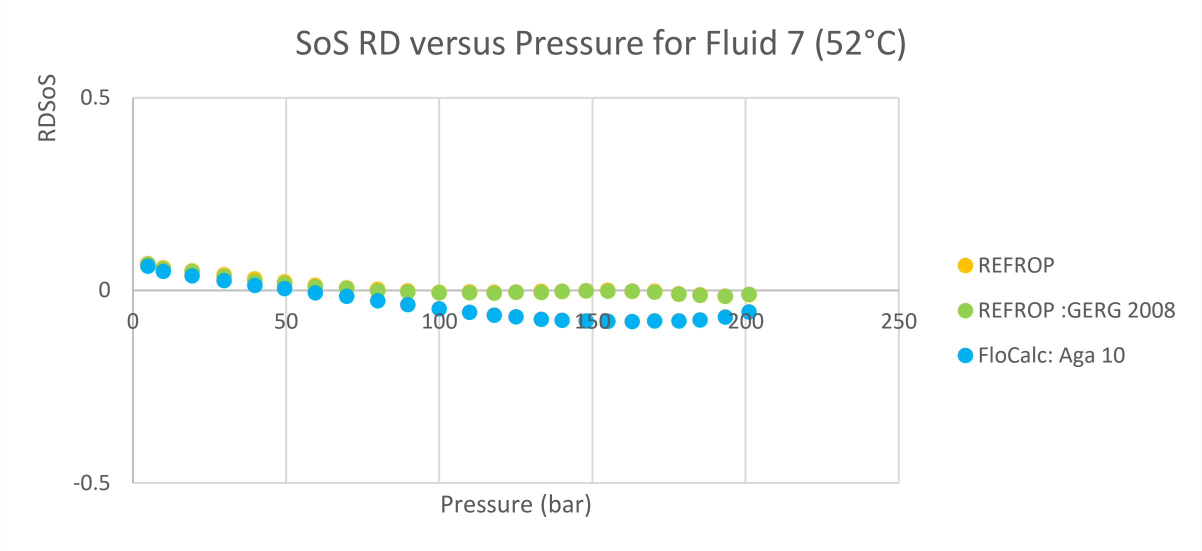

Figure 119: RD SoS versus Pressure for Fluid 7 (52°C)

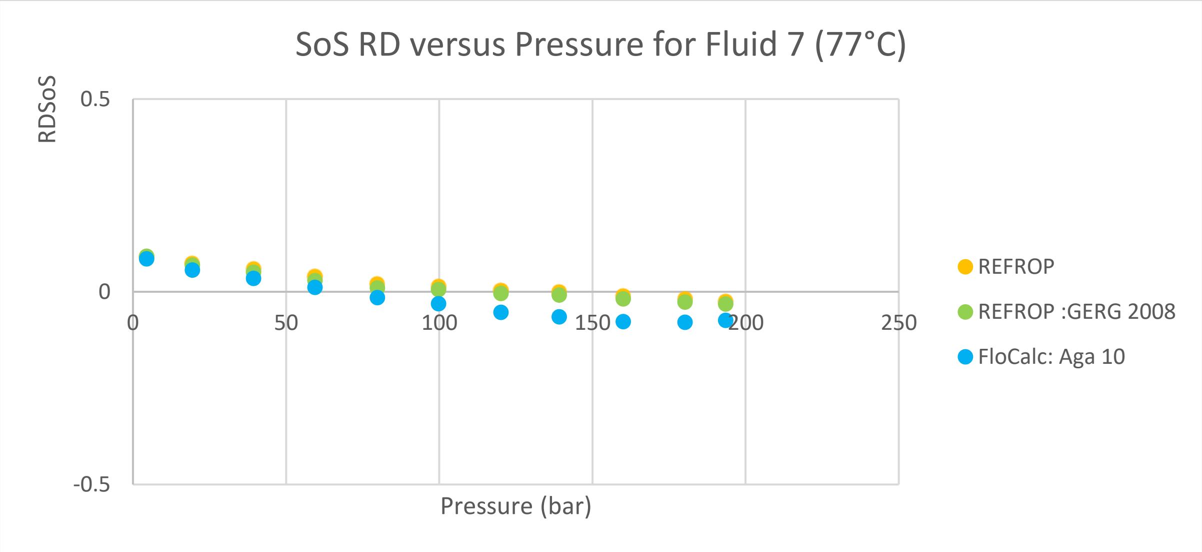

Figure 120: RD SoS versus Pressure for Fluid 7 (77°C)

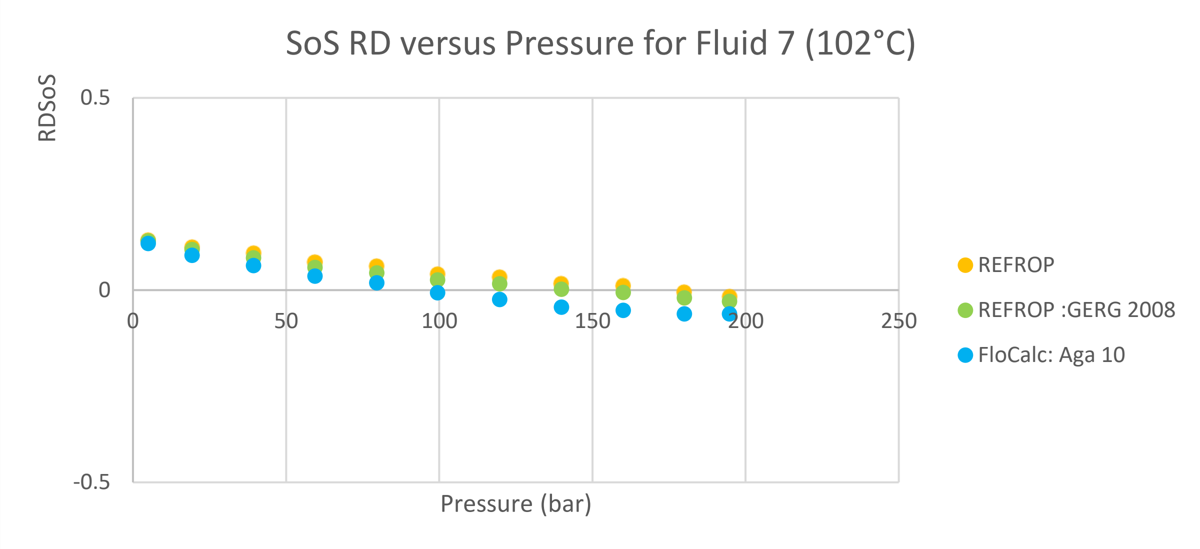

Figure 121: RD SoS versus Pressure for Fluid 7 (102°C)

EoS	AAD SoS at (5 up to 200 bar)				
	0 °C	27°C	52°C	77°C	102 °C
REFPROP	**0.048**	**0.0207**	0.016	0.032	0.054
GERG	0.051	0.0211	**0.015**	**0.031**	**0.048**
AGA 10	0.083	0.068	0.053	0.053	0.053

Table 47: Fluid 7 AAD SoS for each EoS

7.3 Discussion

This section discusses the analysis of each fluid, highlighting the main outcomes by examining the relationship between relative deviation (RD) and average absolute deviation (AAD) under defined process conditions. It also compares the performance of different EoS models and evaluates the influence of each mixture on density and SoS.

7.3.1 Density

For hydrogen–natural gas blends (3–20% H_2, Fluids 1–5), the pressure and temperature ranges included in this study are inconsistent, as they depend on the availability of experimental data. The compositions of fluids 2–5 were obtained from the dataset "Specification for Natural Gas Mixtures with H_2 (Brand New Dataset)" shown in Table 3 of the FluidProp help file provided by HyCCS Tech. The analysis of fluids 2–5 and the natural gas mixture without H_2 produced results that were inconsistent with what KELTON would expect to see. This could potentially be due to experimental uncertainty associated with the density measurements from the test equipment employed in these experiments. Furthermore, the use of nominal rather than fully detailed compositions from the HYCCS Tech database would introduce systematic bias into the calculations. Therefore, fluids 2-5 results were excluded from this report.

External resources were used to assess the EoS performance on different H_2 blends in Fluids 1a, 3a, 4a, and 5a. The results were produced using experimental data from the study "Density Characterization of Hydrogen–Blended Natural Gas Using a Single-Sinker Densimeter." The analyses produced results that were consistent with KELTON's expectations, thereby confirming the validity of the approach.

For fluids (1a, 3a, 4a and 5a), pressure is up to 100 bar and verified at 0°C, 20°C and 50°C.

As for binary mixtures of CH_4 and up to 20% H_2 shown in fluids 6-10, the experimental data has a wide variety allowing for a pressure range of up to 200 bar and temperature from -33°C to around 100°C. Also, more EoS models were considered for the simplicity of the binary mixture of CH_4-H_2.

It is worth noting that, the below statements are generic data analysis of the trend of RDρ density vs. pressure at different temperatures:

Looking at Fluids 1 and 1a, which represent 3% H_2 blends, the performance across multiple EoS models (GERG, Span–Wagner, and REFPROP) is similar, with all AADρ values ≤ 0.1%. For Fluid 1a, GERG appears to have a slight advantage over the pressure range of 30 to 100 bar, while in Fluid 1, AGA 8 shows a slight advantage across the pressure range of 10 to 200 bar.

Fluids 3a, 4a, and 5a represent natural gas mixtures with 10%, 15%, and 20% H_2, respectively. All EoS models (GERG, Span–Wagner, and REFPROP) show similar performance across the experimental process conditions. For Fluids 3a and 5a, AGA 8 performs best at 0°C and 50°C, corresponding to the lowest and highest points of the available experimental datasets, while GERG performs better at 20°C, representing mid-range temperatures. For Fluid 4a, REFPROP provides the best performance at 0°C and 50°C, and GERG shows the lowest deviation at 20°C. The highest deviation recorded across all blends (Fluids 1a, 3a, 4a, and 5a) using the experimental data from "Density Characterization of

Hydrogen–Blended Natural Gas Using a Single-Sinker Densimeter" with the best-performing EoS model occurs for the 3% H_2 blend at 20°C.

For CH_4-dominated mixtures in Fluids 6–9 with low hydrogen content (<20% H_2), deviations are generally smaller across all EoS compared to NG–H_2 mixtures. This is evident when comparing CH_4–20% H_2 (Fluid 9b) with the NG–20% H_2 mixture (Fluid 5), where the AADρ increases from about 0.26% to around 1%. Fluid 9b also shows that multiple EoS models (GERG, Span–Wagner, and REFPROP) perform well depending on the temperature. The three models perform similarly overall, with Span–Wagner giving the best accurate results at lower temperatures 5°C and 25°C before diverging above 75 °C. In summary, AGA 8 can be considered a reliable reference for all Fluids 6–9. However, for Fluid 7, Span–Wagner performs slightly better at lower temperatures (5 °C), while GERG and REFPROP provide slightly better accuracy at higher temperatures (75 °C and 100 °C, respectively).

Overall, AGA 8 is generally accurate at 0°C and 50°C while GERG performs best at mid-range temperatures 20°C. Span–Wagner can be useful for low-temperature CH_4–H_2 mixtures. These findings provide practical guidance for selecting thermodynamic models for hydrogen-blended natural gas applications.

7.3.2 Speed of sound

SoS experimental data for hydrogen–natural gas blends (3–20% H_2, Fluids 1–5), pressure range and temperature included in the study are inconsistent. Similar to the density dataset, the compositions of Fluids 2–5 were obtained from the dataset “Specification for Natural Gas Mixtures with H_2 (Brand New Dataset)” shown in Table 3 of the FluidProp help file provided with HYCCS. The analysis of Fluids 2–5 produced results that were inconsistent with what KELTON would expect to see. This could potentially be due to experimental uncertainty associated with the density measurements from the test equipment employed in these experiments. Furthermore, the use of nominal rather than fully detailed compositions from the HYCCS Tech database would introduce systematic bias into the calculations. Therefore, fluids 2-5 results were excluded from this report.

As for binary mixtures of CH_4 and up to 10 % H_2 shown in fluids 6 and 7, the experimental data show a pressure range of up to 200 bar and temperature from 0°C to around 100°C.

It is worth noting that, the below statements are generic data analysis of the trend of RD SoS vs. pressure at different temperatures:

The results for Fluid 1 show similar performance across all EoS models (GERG, Span–Wagner, and REFPROP), with AAD SoS values of < 0.07% over the full temperature range of –13°C to 77°C and pressures up to 120 bar. GERG performed best at lower temperatures, while REFPROP was the most accurate at temperatures from 27°C to 77°C.

For CH_4-dominated mixtures with 5% and 10% H_2 (Fluids 6 and 7), both REFPROP and GERG perform well, with GERG showing a slight advantage at temperatures above 27 °C. AGA 10 again provides stable predictions but falls short in accuracy compared to the other two models. Notably, the AAD is around 0.02% for CH_4-dominated mixtures with a hydrogen content of 5% and 10% (fluids 6 and 7).

8 Gaps in data

While the analysis provides valuable insight into EoS performance for hydrogen-rich mixtures and hydrogen–natural gas blends, some gaps remain in the experimental datasets:

I. Property Coverage

Density is well-represented and forms the basis of the analysis.

Data for SoS, viscosity, and compressibility factor (Z) is limited, restricting the ability to fully evaluate EoS performance for these parameters.

II. Mixture Composition Coverage

Near-pure hydrogen mixtures (≥90% H_2) are well covered in the current dataset. However, further research is needed into multi-impurity mixtures to better understand their effects on hydrogen-rich mixtures. Additionally, there is value in conducting experiments on low-level hydrogen blends (particularly around 5% H_2) using a single sinker densimeter to expand the coverage and validate measurement accuracy across a wider composition range.

III. Pressure and Temperature Resolution

While coverage is adequate within the target ranges (–10 °C to 40 °C and 0–80 bar), some fluids have fewer data points at certain pressure and temperature steps, which may affect the precision of AAD calculations.

Conclusion:

The existing datasets are sufficient for evaluating EoS performance under near-term operational conditions for hydrogen blending and transport. However, additional measurements for 5% hydrogen blends for density with additional experimental data on other gas properties such as SoS, viscosity and compressibility would enhance the robustness of further studies and provide greater confidence in model selection for all relevant scenarios.

9 References

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