

# Calculation of Compression Factors and Gas Law Deviation Factors Using the Modified SGERG-Equation SGERG-mod-H2

## Technical Report PK 1-5-3

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**Report for the editorial group “gas law deviation factor” (G-AG-1-5-3-1) of the DVGW project team “Gas composition” (PK 1-5-3)**

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## 1 Summary and conclusions

In this paper, the SGERG-88 equation is modified in such a way that the calculation of compression factors and gas law deviation factors is possible for natural gases with higher admixture of hydrogen (see section 3.1). One of the measures to achieve this, is suppressing the so-called “CO correction”. This modified version is termed “SGERG-mod-H2”.

In chapter 4, the equations of state SGERG-88, SGERG-mod-H2, AGA8, and GERG-2008 are compared in detail with experimental compression factors of mixtures containing hydrogen. Furthermore, in chapter 5, a comparison of the different equations of state is given for 5 different natural gases with admixtures of hydrogen between 0 % and 100 mol %.

The analysis of these data leads to the following conclusions:

The equation of state “SGERG-mod-H2” is suitable for the calculation of natural gases with admixtures of up to 100 mol-% H<sub>2</sub>. At pressures up to 50 bar, the deviations from the measured values, as well as from the equation GERG-2008 are less than  $\pm 0.1$  %. For higher pressures up to 100 bar, deviations of up to  $\pm 0.5$  % might occur. Although the equation can theoretically be applied to hydrogen concentrations of up to 100 mol%, numerical problems can occur at very high concentrations of H<sub>2</sub>. Therefore, it is recommended to limit the application range to 30 mol-% H<sub>2</sub> in part 6 of the DVGW G685 [1].

For the equation SGERG-88, for a hydrogen content of up to 10 mol-% and pressures up to 50 bar, an uncertainty of 0.1 % can be expected.

The AGA8 equation and the GERG-2008 equation generally agree better than  $\pm 0.1$ % for the measured values for all data sets in the entire pressure range. It can thus be expected that these equations of state can be used for any desired H<sub>2</sub> fractions without significantly affecting the underlying 0.1% uncertainty of the equations.

## 2 Introduction

There are currently various ongoing activities in the DVGW (German Technical and Scientific Association for Gas and Water) to adapt the gas infrastructure and the gas applications to a higher hydrogen content. In this context, the DVGW technical guidelines shall be reviewed in terms of possible limitations of the concentration of hydrogen and shall be adapted if necessary. Among others, this concerns the DVGW code of practice G 685 [1], which has been revised in August 2020. Part 6 of the G685 describes the determination of the compression factor and the gas law deviation factor which is necessary for the conversion of the volume at measurement conditions to the volume at standard conditions. For this reason, the DVGW Project Group PK 1-5-3 convened the editorial group “Gas law deviation factor” in order to review the determination of the gas law deviation factor according to the DVGW code of practice G685-6, taking into account the admixture of hydrogen.

The background of this work are the equations of state SGERG-88 [2] and AGA8 [3], which are defined as state of the art in the above-mentioned code of practice. They are extensively examined for their suitability to calculate gas mixtures containing hydrogen. The SGERG-88 equation, for which a limitation with respect to the H<sub>2</sub> concentration was known in advance, is modified here in such a way that a calculation of mixtures with hydrogen concentrations of up to 100% is possible. In the following, this modified version will be referred to as “SGERG-mod-H2”. The modifications are explicated in section 3.1.

The validation of the equations of state is based on experimental literature data. In addition, the GERG-2008 equation [4] is used for the comparison. The examination takes place for hydrogen fractions between 0 % and 100 mol %. For hydrogen fractions > 30 mol %, experimental literature data are only available for binary mixtures of methane and hydrogen (CH<sub>4</sub>/H<sub>2</sub>).

## 3 Description of the considered equations of state

At the present time in Germany, volume conversion is essentially based on two equations. Their use is described in the DVGW code of practice G685-6.

The SGERG-88 equation (see section 3.1), which takes into account the calorific value, the density at standard conditions (in short standard density), the CO<sub>2</sub> content, and the H<sub>2</sub> content for the gas properties characterization, is mainly used in regional distribution networks, where the pressure is mostly below 50 bar, usually even below 25 bar.

The AGA8-92DC equation (see section 3.2) requires a complete gas analysis (e.g. 12 components) as input information for characterizing the gas properties. As this information is often not available in regional distribution networks, the use of the AGA8 is currently mainly limited to the gas transport networks.

In addition to the above-mentioned equations, the GERG-2008 equation is also described in this chapter. It requires a complete gas analysis as input information, as well. The GERG-2008 equation is characterized by a very wide range of application regarding the different gas

components and serves as an additional reference for the comparisons given in the chapters 4 and 5.

### 3.1 SGERG-88 and SGERG-mod-H2

The SGERG-88 equation has been developed by Jaeschke et al. [5] for the calculation of compression factors and gas law deviation factors. In 1997, it has been described in the international standard ISO 12213-3 [2]. In the ISO standard, its application is limited to the composition of “Pipeline Quality Gas”, whereby a limit of 10 mol % is defined as a limit for the hydrogen content. Furthermore, the relative density is limited to the range of  $0.55 \leq d \leq 0.80$ ; this corresponds to a range of the density at standard conditions of  $0.711 \text{ kg/m}^3 \leq \rho_n \leq 1,034 \text{ kg/m}^3$ . For some compositions of natural gas, the lower limit of the relative density (or density at standard conditions) results in a maximum hydrogen content of 5 mol %. The limits given in the ISO standard comply with the range of application which is expected at the transport of natural gas. Back then, the admixture of renewable hydrogen surely has not been considered. The limits of the ISO standard were incorporated in the DVGW code of practice G685-6. [1].

In addition, the Annex B.5 of the ISO 12213-3 describes consistency checks by the equations B.43 ( $d > 0,55 + 0,97 \cdot x_{\text{CO}_2} - 0,45 \cdot x_{\text{H}_2}$ ) and B.46 ( $d > 0,55 + 0,4 \cdot x_{\text{N}_2} - 0,97 \cdot x_{\text{CO}_2} - 0,45 \cdot x_{\text{H}_2}$ ). These also result in a limitation of the maximum content of hydrogen.

An additional influence of the calculation which depends on the hydrogen content is the so-called “carbon monoxide correction” (CO correction). It is assumed that, if hydrogen is present, carbon monoxide also exists in the mixture, in a fixed relation to the hydrogen content, which is 0.0964. This is expressed by equation B.2 in appendix B of the ISO document ( $x_{\text{CO}} = 0,0964 \cdot x_{\text{H}_2}$ ). The CO content is considered in the calculation, using the corresponding virial coefficients of CO. The described correction is based on the assumption that the hydrogen is generated as a component of coke oven gas, and that in this process, carbon monoxide is generated in the above-mentioned ratio. In case of pure hydrogen, produced for example by water electrolysis, this correction of course does not make sense and is expected to cause a deterioration of the calculation results. As the feed-in of coke oven gas into gas grids does not occur anymore, the CO correction can be omitted.

In order to enable the calculation of compression factors and gas law deviation factors based on the SGERG equation also at a higher content of hydrogen, the existing algorithm has been modified in the scope of this work, in such a way that the above-mentioned limitations are abolished. Therefore, the inquiry of the range of application, the consistency checks, and the carbon monoxide correction are omitted. These modifications were made in the original Fortran code which is published in Appendix G of ISO 12213-3 (see Appendix E). For executing the calculations, the software Gas Calc ([www.GasCalc.de](http://www.GasCalc.de)) is used. In the following, the SGERG equation, modified in this way, is denoted as **SGERG-mod-H2**.

## 3.2 AGA8

The equation AGA8-92DC, in the following simply denoted as AGA8 - has been developed by Starling et al. ([6] [7]) for the calculation of natural gas and similar mixtures in the gaseous state and is described in the standard ISO 12213-2 [3]. Besides to the SGERG-88 equation, it has also been included in the DVGW code of practice G685-6 [1]. The AGA8 equation includes 21 components of natural gas for characterizing the gas composition: methane, nitrogen, carbon dioxide, ethane, propane, n-butane, iso-butane, n-pentane, iso-pentane, n-hexane, n-heptane, n-octane, n-nonane, n-decane, hydrogen, oxygen, carbon monoxide, water, hydrogen sulfide, helium, and argon. In the ISO standard, as in the case of SGERG-88, the content of hydrogen is limited to 10 mol% corresponding to the specification of "Pipeline Quality Gas" (see section 3.1).

For the examinations in the frame of this work, the AGA8 equation could be used for a hydrogen content between 0 % and 100 % by omitting the inquiry for the application range. The calculations have been performed using the software GasCalc ([www.GasCalc.de](http://www.GasCalc.de)).

## 3.3 GERG-2008

The GERG-2008 equation was first published by Kunz et al. in 2007 with the denotation GERG-2004. In 2012, an extended version called GERG-2008 was published by Kunz and Wagner [4] In 2015, it was described in the international standard ISO 20765 [8].

The development of the equation GERG-2008 [4] was based on a data bank with more than 125,000 experimental data for various thermodynamic properties in different phases. The experimental data comprise pure substances, binary mixtures as well as a big variety of multi-component mixtures. The equation of state GERG-2008 considers the same 21 natural gas components as the AGA8 equation (see section 3.2). The equation is valid over a wide temperature and pressure range and comprises the gaseous and the liquid state as well as liquid-gas-equilibria and the supercritical range. In the frames of this work, the GERG-2008 equation is mainly used as a reference for the comparison with the equations SGERG-88, SGERG-mod-H2, and AGA8.

## 4 Comparison of the equations of state with measurement results

In the following, the equations of state described in chapter 3 are examined based on experimental data for their suitability to describe mixtures containing hydrogen. The analysis is based on measurement values of compression factors of natural gases with admixtures of hydrogen and binary mixtures of methane and hydrogen.

Besides to the equations SGERG-88 [2] and SGERG-mod-H2 (introduced in this paper), the equations AGA8 [3] and GERG-2008 [4] are considered as well. For comparison, the relative deviations of the compression factors are plotted in diagrams as a function of pressure (see **Figure 4-1**, **Figure 4-2**, **Figure 4-3**). Thereby, the equation GERG-2008 is chosen as the reference, which leads to the following equation for the relative deviation:

$$\delta Z_{\text{GERG-2008}} = 100 \cdot \frac{Z - Z_{\text{GERG-2008}}}{Z_{\text{GERG-2008}}} \quad (4-1)$$

In addition, the highest deviations of the respective equation from the experimental data are summarized in tables (see **Table 4-2**, **Table 4-4**, **Table 4-6**). Thereby, the relative deviation from the measured value is determined as follows:

$$\delta Z_{\text{exp}} = \left| 100 \cdot \frac{Z - Z_{\text{exp}}}{Z_{\text{exp}}} \right| \quad (4-2)$$

In the tables, the maximum deviations are given as absolute values for the pressure ranges 0 to 50 bar and 0 to 100 bar. The pressure range 0 to 50 bar comprises the pressure range of most ptz volume conversion devices using the SGERG-88 calculation method.

The deviations depicted in the following are also a good approximation for the uncertainty of the gas law deviation factors  $K (= Z / Z_n)$ , because the uncertainty of the compression factor at standard conditions  $Z_n$  is negligible.

### 4.1 Comparison for natural gases with admixtures of hydrogen (high-precision measurement results of Ruhr University Bochum)

The “2-sinker densimeter” developed by Ruhr university Bochum (RUB) with a measurement uncertainty of 0.02%, is regarded as the most accurate method for density and the compression factors determination of gas mixtures.

In the last decades, this method has been used for the measurement of 4 different natural gases with admixtures of hydrogen. An overview of the examined mixtures and data sets is given in **Table 4-1**. The mixture M1 with a hydrogen content of approximately 8 mol-% was measured in 1993 in the frame of a contract with the Ruhrgas AG [9] and is also included in the GERG-Monograph TM15 [10]. The mixtures NG1, NG2, and NG3 with a hydrogen content of approximately 5, 10, and 30 mol-% were measured in 2014 in the framework of a DVGW research project [11]. The results were published in 2017 by Richter et al. [12]. The compositions of the gas mixtures under examination are given in Annex C.



In the above-mentioned publication, the measured density is given together with the corresponding values for pressure and temperature. In addition, the molar mass is given for every gas mixture, which can be determined for a series of measurements by extrapolation of the density to the pressure  $p = 0$  bar. Based on this result, the corresponding compressibility factors can be calculated using the following relation:

$$Z = \frac{p \cdot M}{\rho \cdot R \cdot T} \quad (4-3)$$

The comparison of the different equations of state with the experimental data is depicted in **Figure 4-1** to **Figure 4-4**. **Table 4-2** contains an overview of the highest absolute deviations of the respective equation from the measured values.

Over the whole pressure range and for the four examined mixtures, the results show a very good agreement for both the GERG-2008 equation and the AGA8 equation. The highest deviation for the mixture NG2 is 0.064 % for the GERG-2008-equation (at 0 °C and 60.3 bar) and 0.051 % for the AGA8 equation (at 0 °C and 80.4 bar). In all other cases, the deviations are less than  $\pm 0.05$  %.

The SGERG-88 equation is suitable for the mixtures M1, NG1, and NG2. In the case of the mixture NG2, this requires omitting the inquiry of the application range ( $x_{H_2} \leq 10$  mol%). The mixture NG3, cannot be calculated due to the consistency checks described in section 3.1. For the pressure range between 0 bar and 50 bar, the SGERG-88 equation also agrees well with the measurements. In all cases, the deviation is less than  $\pm 0,1\%$ ; the highest deviation of 0.099 % has been found for the mixture NG2 (at 0 °C and 40.2 bar). For pressures higher than 50 bar, deviations of up to 0.4 % occur. The highest deviation of 0.399 % is found for the mixture NG2 (at 0 °C and 80.4 bar).

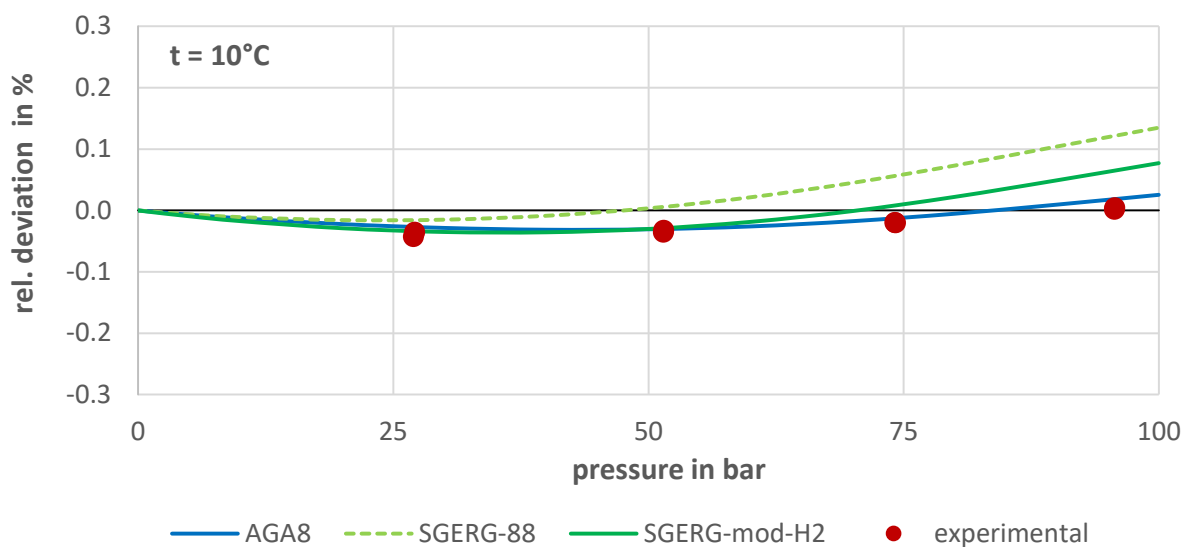
With the SGERG-mod-H2 equation, calculations are possible without problems for all 4 mixtures. In the pressure range between 0 bar and 50 bar, there is a very good agreement with the measured values. Generally, the deviations are less than  $\pm 0,05\%$ , except for the mixtures NG1 and NG2 at 0 °C and approximately 40 bar, with deviations of 0.055 % and 0.054 %. It becomes apparent that omitting the "CO correction" (see section 3.1) leads to better reproduction of experimental data, compared to the SGERG-88 equation. For pressures above 50 bar, deviations up to approximately  $\pm 0,3\%$  occur. The highest deviation of 0.306 % is found for the mixture NG2 (at 0°C and 80.4 bar). However, for the mixture NG3 with the highest hydrogen content of 30.47 mol%, the deviations are below 0.1 % in the whole pressure range. It shall be noted that in general, the SGERG equation leads to an increased uncertainty ( $>0.1$  %) in the pressure range of approximately 80 to 100 bar, regardless of hydrogen admixtures.

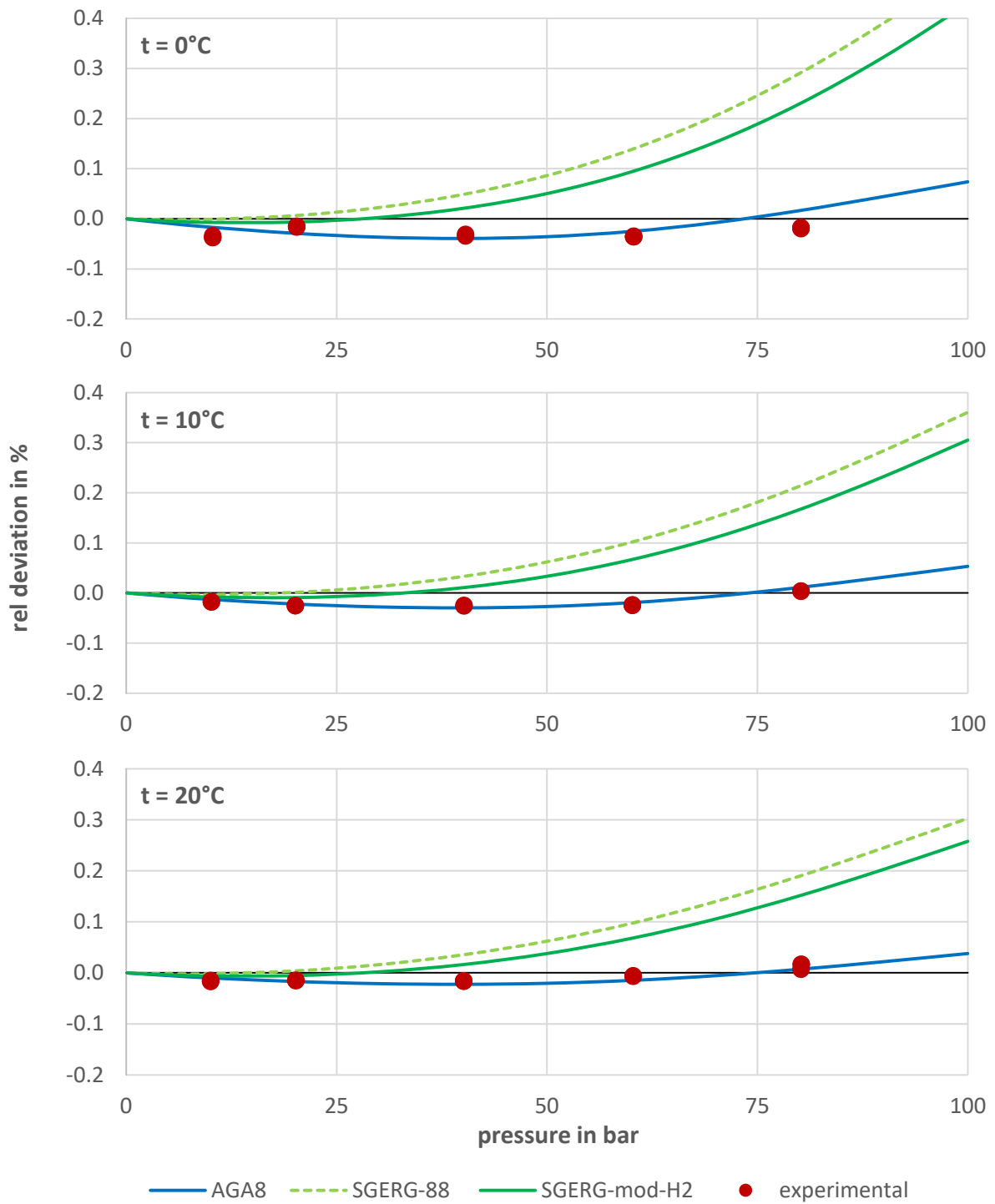
**Table 4-1:** Overview of experimental data sets for the assessment (for GC analysis see Annex C).

Mixture	Method	Number of data points	$T$ °C	$p$ bar	$x_{H_2}$ mol%
M1	2-sinker densimeter	8	10	27 – 96	8.11
NG1	2-sinker densimeter	37	0, 10, 20	10 – 81	5.37
NG2	2-sinker densimeter	36	0, 10, 20	10 – 81	10.41
NG3	2-sinker densimeter	13	10	10 – 81	30.47

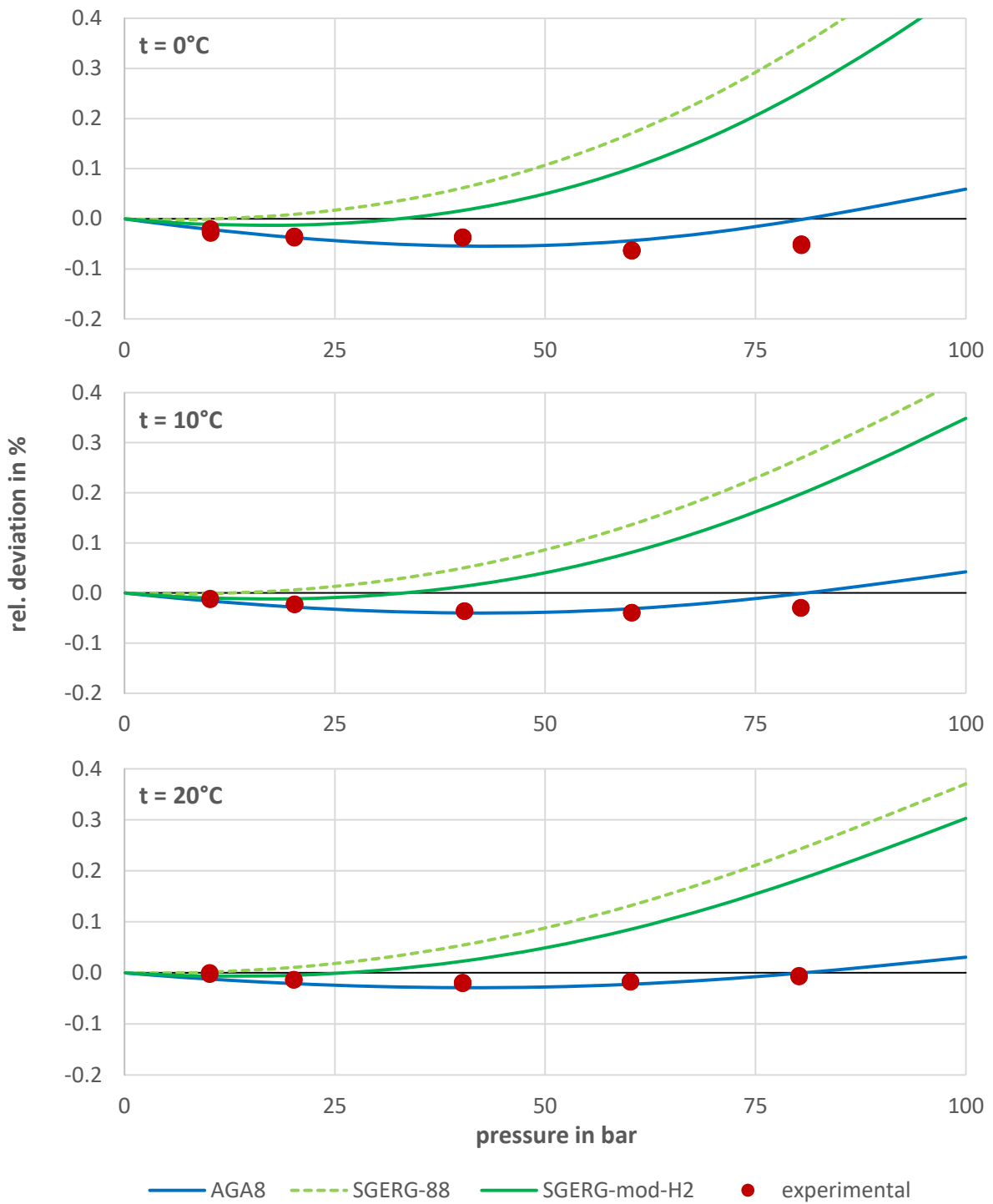
**Table 4-2:** Maximum absolute deviation of compression factors calculated with different equations of state from experimental values for data sets M1, NG1, NG2 and NG3.

Mixture	t °C	SGERG-88		SGERG-mod-H2		AGA8		GERG-2008	
		0-50 bar	0-100 bar	0-50 bar	0-100 bar	0-50 bar	0-100 bar	0-50 bar	0-100 bar
<b>M1</b>	10	0.026	0.120	0.008	0.063	0.015	0.016	0.042	0.042
	0	0.083	0.311	0.055	0.250	0.020	0.036	0.037	0.037
<b>NG1</b>	10	0.058	0.210	0.036	0.163	0.005	0.007	0.025	0.025
	20	0.052	0.183	0.033	0.145	0.007	0.010	0.017	0.017
<b>NG2</b>	0	0.099	0.399	0.054	0.306	0.017	0.051	0.038	0.064
	10	0.086	0.298	0.049	0.227	0.006	0.028	0.036	0.039
	20	0.074	0.249	0.043	0.190	0.013	0.013	0.020	0.020
<b>NG3</b>	10	calculation not possible		0.014	0.061	0.038	0.042	0.025	0.025

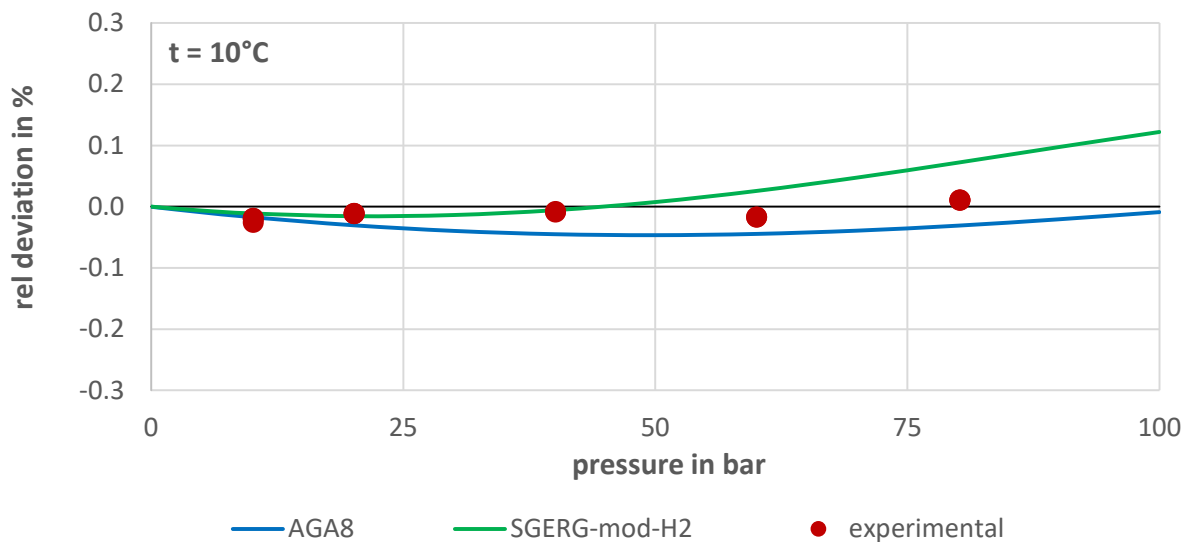
**Figure 4-1:** Comparison of measured and calculated compression factors (AGA8, SGERG-88, SGERG-mod-H2, GERG-2008) for mixture **M1** ( $x_{H_2} = 8,11$  mol%) at 10°C. The diagram shows relative deviations with respect to the GERG-2008 equation.



**Figure 4-2:** Comparison of measured and calculated compression factors (AGA8, SGERG-88, SGERG-mod-H2, GERG-2008) for mixture **NG1** ( $x_{\text{H}_2} = 5,32 \text{ mol\%}$ ) at  $10^\circ\text{C}$ . The diagram shows relative deviations with respect to the GERG-2008 equation.



**Figure 4-3:** Comparison of measured and calculated compression factors (AGA8, SGERG-88, SGERG-mod-H2, GERG-2008) for mixture **NG2** ( $x_{\text{H}_2} = 10,41$  mol%) at  $10^\circ\text{C}$ . The diagram shows relative deviations with respect to the GERG-2008 equation.



**Figure 4-4:** Comparison of measured and calculated compression factors (AGA8, SGERG-88, SGERG-mod-H2, GERG-2008) for mixture **NG3** ( $x_{\text{H}_2} = 30,47 \text{ mol\%}$ ) at  $10^\circ\text{C}$ . The diagram shows relative deviations with respect to the GERG-2008 equation.

## 4.2 Comparison of natural gases with admixtures of hydrogen (GERG data base TM7)

The GERG data bank TM7 (Jaeschke *et al.* [13], 1997) comprises a total of 36.239 experimental compression factors of pure substances, binary mixtures, multicomponent mixtures, and natural gases. In this section, the data sets of natural gases with admixtures of hydrogen are analysed. An overview of the considered data sets is given in **Table 4-3**. The highest hydrogen content found in these data is 9.49 mol%. The measurements were carried out between 1980 and 2000 by the former Ruhrgas AG using the Burnett method as well as the optical method. For both methods, the specified measurement uncertainty is 0.1 %. Therefore, the results given in the following text are not of the same significance as the results given in section 4.1. A graphical representation of the relative deviations is given in the Annexes A1 to A8.

For the equations AGA8 and SGERG-2008, the results show a very good compliance with the measured values, which is in most cases within  $\pm 0,1\%$ . Only in particular cases, deviations exceeding 0.1 % are found. In case of the AGA8 equation, the highest deviations amount to 0.143 % for the mixture N67 (at  $0^\circ\text{C}$  and 91.6 bar) and 0.192 % for the mixture N70 (at  $0^\circ\text{C}$  and 91.6 bar). For the GERG-2008 equation, the maximum deviation amounts to 0.143 %, and the same is obtained for the mixture N70 (at  $0^\circ\text{C}$  and 91.6 bar). It shall be pointed out once more that these deviations may be caused by the general uncertainty of the equations as well as by the measurement uncertainty and are not necessarily caused by the hydrogen content.

For the equations SGERG-88 and SGERG-mod-H2, the agreement with the measured values is very good as well. In the whole pressure range, the deviations are usually less than  $\pm 0,1\%$ . Only in particular cases, deviations of more than 0.1 % are found. In case of the SGERG-88, the highest deviation is 0.127 % for the mixture N70.

**Table 4-3:** Overview of experimental data sets for the assessment (for GC analysis see Annex C).

Mixture	Method	Number of data points	$t$ °C	$p$ bar	$x_{H_2}$ mol%
N67	Burnett	68	0 – 30	4 – 92	2.31
N68	Burnett	69	0 – 30	4 – 92	4.19
N69	Burnett	70	0 – 30	4 – 92	9.39
N70	Burnett	68	0 – 30	4 – 92	2.28
N71	Burnett	70	0 – 30	4 – 92	4.22
N72	Burnett	67	0 – 30	4 – 92	9.49
N73	Burnett	24	36.85	5 – 100	9.49
N74	Optik	100	-3.15 – 56.85	4 – 100	9.49

**Table 4-4:** Maximum absolute deviation of compression factors calculated with different equations of state from experimental values for data sets N67 to N74.

Mixture	$t$ °C	SGERG-88		SGERG-mod-H2		AGA8		GERG-2008	
		0-50 bar	0-100 bar	0-50 bar	0-100 bar	0-50 bar	0-100 bar	0-50 bar	0-100 bar
N67	0	0.032	0.074	0.015	0.039	0.030	0.143	0.071	0.097
	10	0.029	0.071	0.018	0.045	0.037	0.129	0.072	0.093
	20	0.038	0.086	0.027	0.065	0.042	0.111	0.071	0.090
	30	0.032	0.081	0.033	0.063	0.031	0.076	0.048	0.066
N68	0	0.016	0.047	0.016	0.016	0.017	0.059	0.051	0.063
	10	0.020	0.016	0.043	0.043	0.026	0.026	0.025	0.025
	20	0.015	0.018	0.023	0.023	0.014	0.014	0.028	0.028
	30	0.010	0.027	0.024	0.024	0.023	0.023	0.023	0.023
N69	0	0.024	0.063	0.056	0.135	0.049	0.049	0.014	0.032
	10	0.020	0.072	0.054	0.126	0.038	0.038	0.019	0.035
	20	0.030	0.069	0.059	0.113	0.047	0.047	0.015	0.043
	30	0.015	0.029	0.025	0.067	0.018	0.025	0.019	0.019
N70	0	0.064	0.127	0.046	0.093	0.061	0.192	0.102	0.143
	10	0.036	0.081	0.022	0.055	0.044	0.137	0.079	0.106
	20	0.041	0.099	0.029	0.078	0.044	0.122	0.073	0.099
	30	0.014	0.070	0.016	0.052	0.013	0.063	0.025	0.053
N71	0	0.013	0.022	0.021	0.043	0.017	0.026	0.049	0.049
	10	0.045	0.045	0.070	0.070	0.052	0.052	0.013	0.029
	20	0.018	0.018	0.031	0.039	0.020	0.024	0.035	0.035
	30	0.023	0.023	0.025	0.026	0.023	0.029	0.019	0.024
N72	0	0.014	0.039	0.051	0.111	0.042	0.042	0.020	0.020
	10	0.012	0.038	0.041	0.093	0.024	0.024	0.024	0.024
	20	0.042	0.046	0.071	0.084	0.059	0.059	0.026	0.045
	30	0.021	0.049	0.046	0.087	0.038	0.040	0.011	0.033
N73	36.85	0.009	0.014	0.017	0.046	0.008	0.008	0.018	0.019
N74	-3.15	0.039	0.058	0.011	0.054	0.011	0.101	0.059	0.075
	6.85	0.023	0.036	0.018	0.065	0.012	0.068	0.047	0.066
	16.85	0.004	0.034	0.033	0.080	0.019	0.019	0.016	0.020
	36.85	0.012	0.047	0.032	0.083	0.023	0.035	0.009	0.024
	56.85	0.010	0.043	0.036	0.082	0.004	0.006	0.020	0.020

In case of the SGERG-mod-H2, the highest deviation is 0.135 % (at 0 °C and 91.6 bar) for the mixture N69 (at 0 °C and 92.3 bar). In the pressure range between 0 bar and 50 bar, the deviation amounts to less than  $\pm 0,1\%$  in all cases - usually even less than  $\pm 0,05\%$ , which is partly even better than for the equations AGA8 and GERG-2008. In this context, it shall be noted that the considered data sets in the GERG data bank TM7 have been part of the database which was used for the development of the SGERG equation.

### 4.3 Comparison for binary mixtures of methane and hydrogen (GERG data base TM7)

Since there are no published measurement values for natural gas with admixtures of more than 30 % hydrogen, additionally the binary mixtures of CH<sub>4</sub> and H<sub>2</sub>, with the hydrogen content of up to 75 mol% will be observed. Thereby, it should be noted that the range of application of the SGERG-88 equation is limited to natural gas.

The results show a very good agreement with the measured values for both the AGA8 equation and the GERG-2008 equation. In all cases, the deviations are less than  $\pm 0,1\%$ ; usually less than  $\pm 0,05\%$ . This proves that by using these equations of state, calculations for mixtures with arbitrary hydrogen concentrations in the range of 0 to 100 % are possible.

For the SGERG-mod-H2 equation, there is also a good agreement with the measurement results, at least in the pressure range up to 50 bar. In this range, the maximum deviation is 0.139 % for the mixture B6 (at 1.85 °C and 45 bar). Calculation of these mixtures is not possible with the SGERG-88 equation.

**Table 4-5:** Overview of experimental data sets – binary mixtures methane-hydrogen (the mole fraction of methane is determined by  $x_{\text{CH}_4} = 100 \text{ mol\%} - x_{\text{H}_2}$ ).

Mixture	Method	Number of data points	<i>t</i> °C	<i>p</i> bar	<i>x</i> <sub>H<sub>2</sub></sub> mol%
B1	Burnett	68	0 – 30	4 – 92	15.020
B2	Optik	69	0 – 30	4 – 92	15.020
B3	Optik	70	0 – 30	4 – 92	25.309
B4	Burnett	68	0 – 30	4 – 92	50.266
B5	Optik	70	0 – 30	4 – 92	50.266
B6	Burnett	67	0 – 30	4 – 92	74.940
B7	Optik	85	10 – 20	30 – 70	74.940

**Table 4-6:** Maximum absolute deviation of compression factors calculated with different equations of state from experimental values for data sets B1 to B7.

Mixture	t °C	SGERG-88		SGERG-mod-H2		AGA8		GERG-2008	
		0-50 bar	0-100 bar	0-50 bar	0-100 bar	0-50 bar	0-100 bar	0-50 bar	0-100 bar
<b>B1</b>	0			0.032	0.202	0.022	0.054	0.018	0.018
	20	calculation not possible		0.029	0.159	0.014	0.022	0.011	0.022
	40			0.039	0.163	0.006	0.006	0.016	0.037
<b>B2</b>	0	calculation not possible		0.039	0.224	0.025	0.065	0.020	0.022
	40			0.058	0.183	0.013	0.019	0.007	0.019
<b>B3</b>	-3			0.039	0.154	0.053	0.104	0.048	0.062
	17	calculation not possible		0.043	0.143	0.035	0.068	0.027	0.027
	37			0.071	0.185	0.032	0.069	0.019	0.031
	57			0.060	0.171	0.015	0.023	0.017	0.017
<b>B4</b>	2			0.070	0.191	0.036	0.037	0.017	0.017
	37	calculation not possible		0.009	0.055	0.007	0.007	0.011	0.018
	47			0.016	0.017	0.007	0.007	0.016	0.020
	57			0.030	0.030	0.019	0.019	0.019	0.022
<b>B5</b>	-3			0.065	0.220	0.045	0.068	0.021	0.030
	17	calculation not possible		0.038	0.148	0.043	0.043	0.041	0.041
	37			0.012	0.057	0.016	0.023	0.010	0.010
	57			0.044	0.044	0.037	0.037	0.035	0.035
<b>B6</b>	2			0.131	0.311	0.012	0.015	0.032	0.038
	37	calculation not possible		0.047	0.240	0.010	0.029	0.013	0.013
	57			0.009	0.076	0.008	0.017	0.006	0.008
<b>B7</b>	-3			0.111	0.369	0.054	0.054	0.047	0.047
	17	calculation not possible		0.087	0.330	0.024	0.024	0.028	0.028
	37			0.044	0.203	0.015	0.027	0.016	0.016
	57			0.024	0.131	0.023	0.029	0.017	0.017



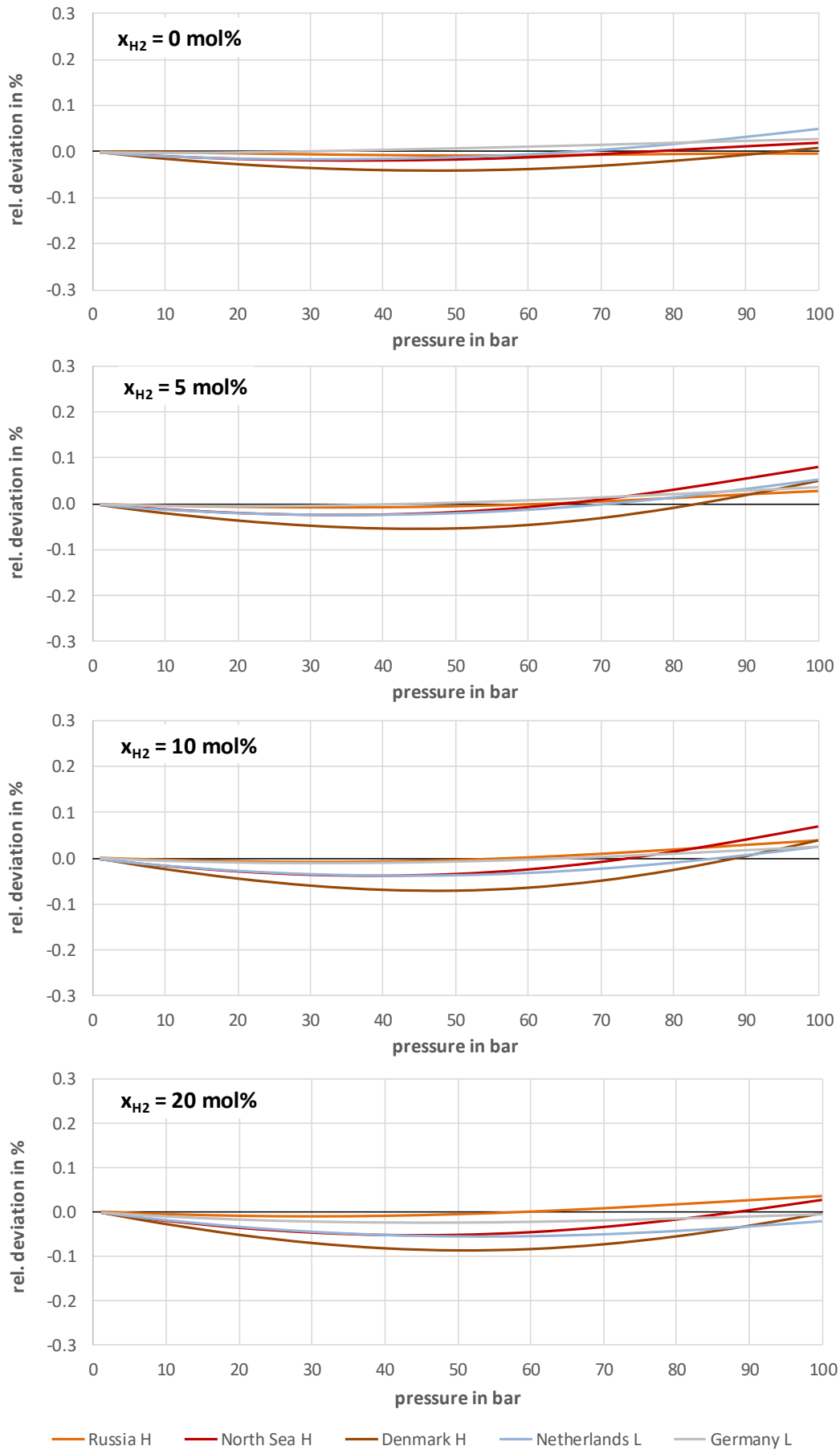
## 5 Comparison between the equations of state

In this chapter, a comparison of the equations of state is carried out based on 5 different natural gases, whereby the hydrogen content in the analysis varies between 0 % and 100 mol%. The composition of the respective natural gases is given in table A.2 of the G260 [14]. The calculations have been carried out at  $t = 10^{\circ}\text{C}$  for pressures up to 100 bar.

For the comparison of the equations of state, the GERG-2008 equation has been chosen as reference. **Figure 5-1** and **Figure 5-2** show the relative deviations of the AGA8-equation in comparison to the GERG-2008 equation. **Figure 5-3** and **Figure 5-4** show the relative deviations of the equations SGERG-88 and SGERG-mod-H2 to the equation GERG-2008.

The results demonstrate that the equations AGA8 and GERG-2008 are in very good accordance. For any contents of hydrogen, and in the whole pressure range, the relative deviations are less than  $\pm 0.1$  %.

For pressures up to 50 bar, the SGERG-mod-H2 equation is also in accordance with the GERG-2008 equation within  $\pm 0.1$  % for any  $\text{H}_2$  content. For pressures above 50 bar, deviations up to 0.44 % occur (for natural gas “North Sea H” with 10 mol% hydrogen at 100 bar). For the equation SGERG-88, the deviations at hydrogen admixtures of up to 10 % are usually less than 0.1 % as well. Only for the natural gas “North Sea H” with 10 mol% hydrogen, there is a deviation of 0.117 % at 50 bar.



**Figure 5-1:** Relative deviations of the **AGA8 equation** from the **GERG-2008 equation** for different natural gases ( $t = 10^\circ\text{C}$ ,  $x_{H_2} = 0\text{--}20\text{ mol\%}$ ).

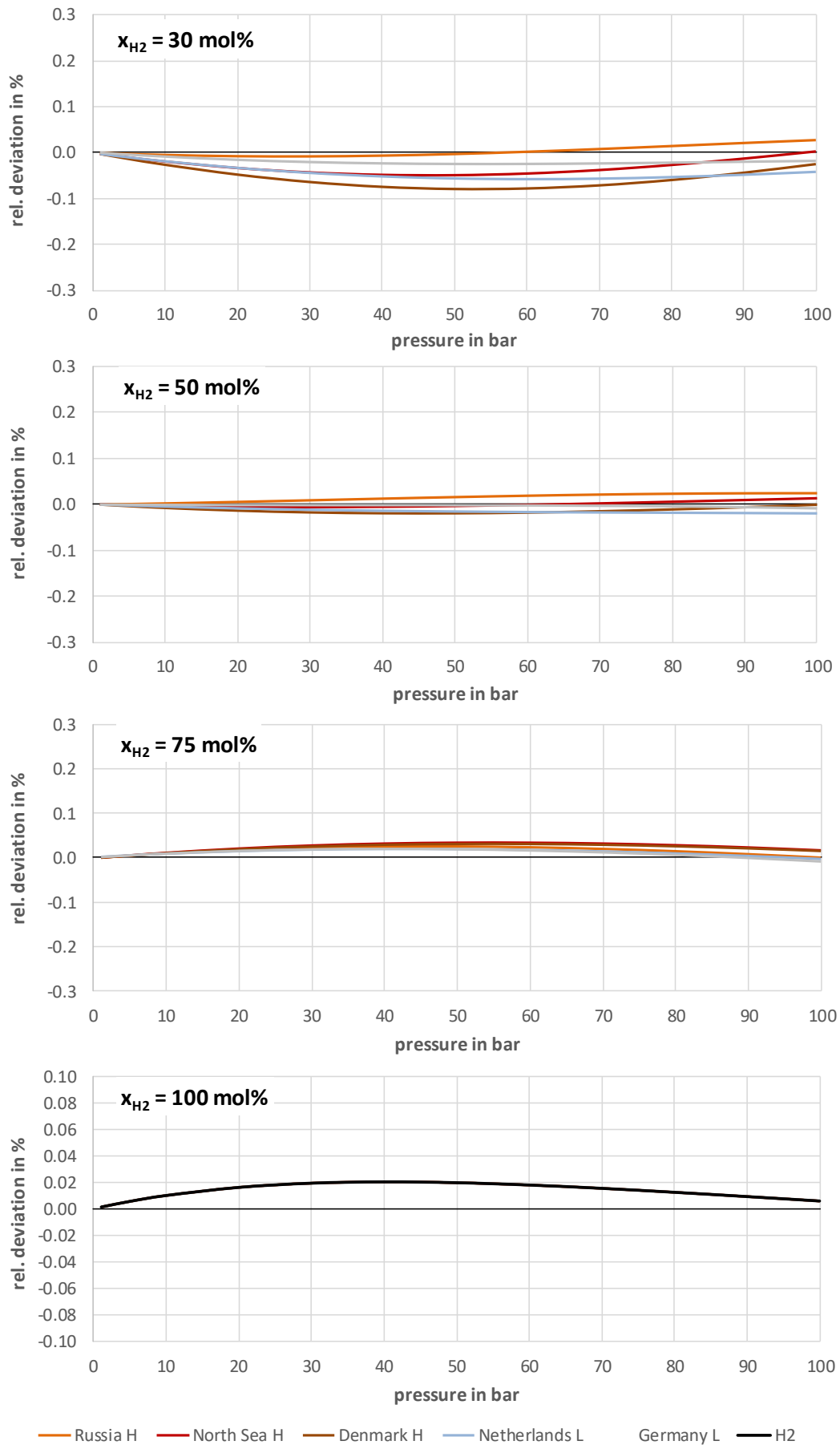
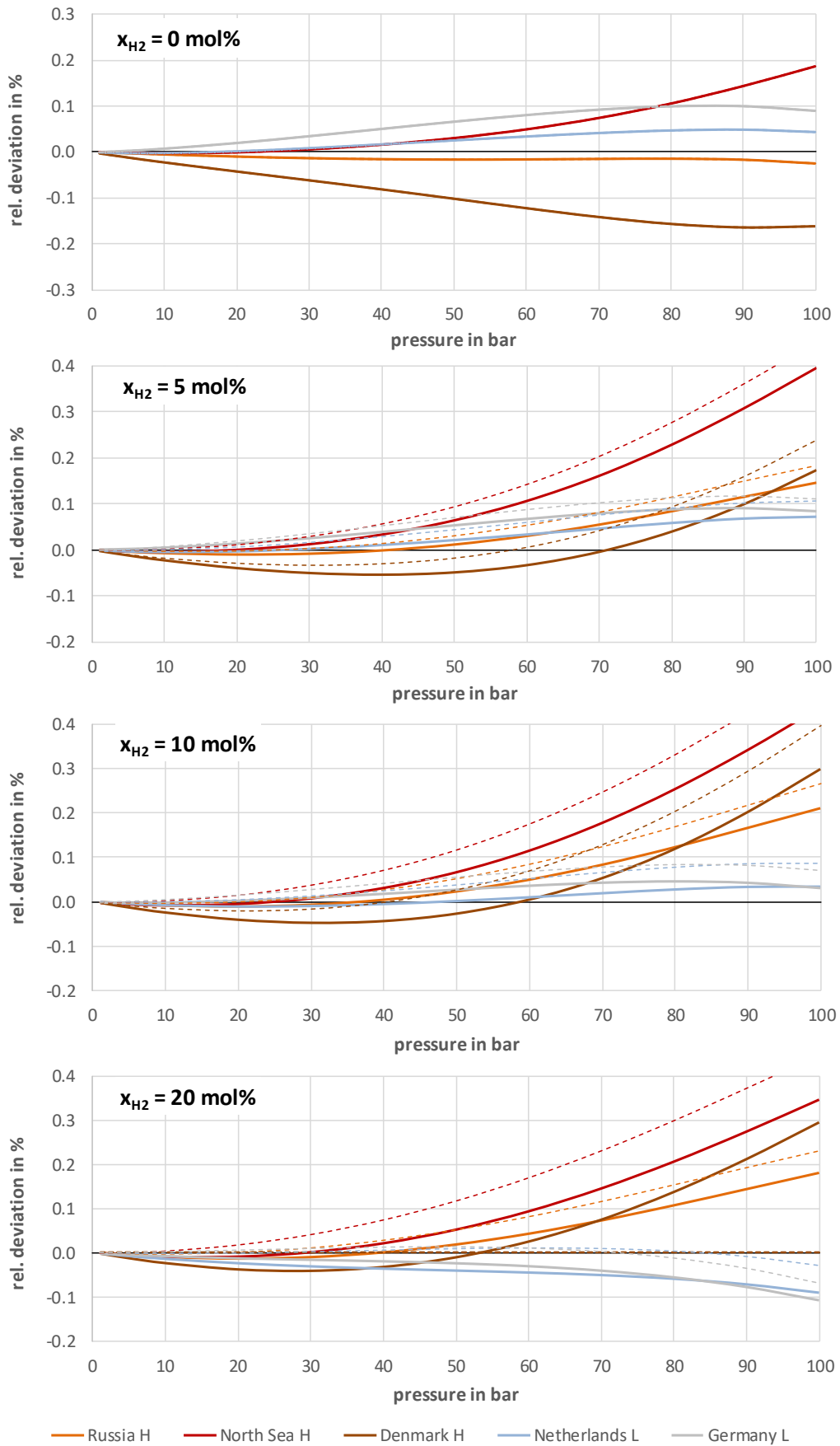
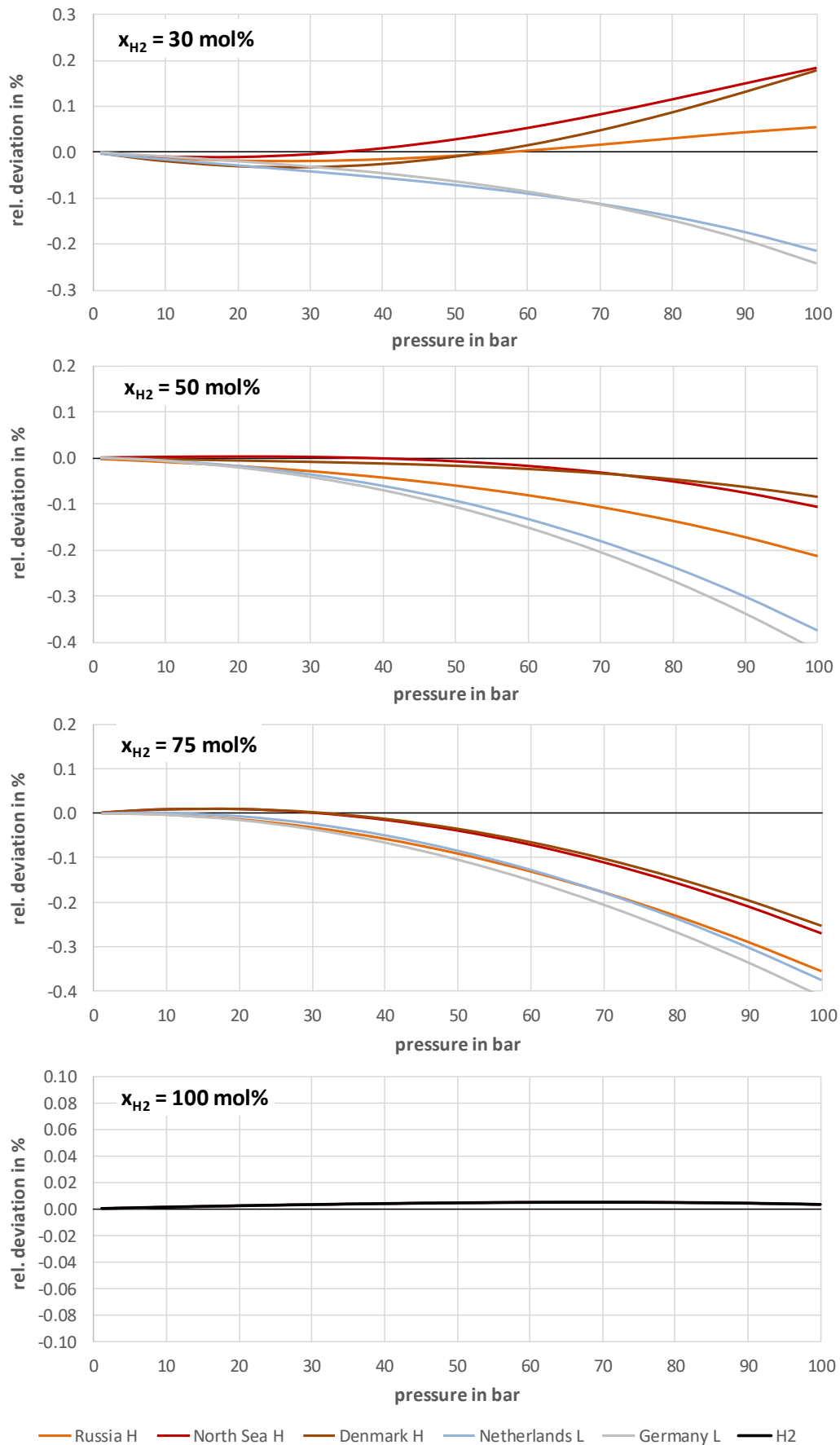


Figure 5-2: Relative deviations of the AGA8 equation from the GERG-2008 equation for different natural gases ( $t = 10^\circ\text{C}$ ,  $x_{H_2} = 30\text{--}100 \text{ mol\%}$ ).



**Figure 5-3:** Relative deviations of the SGERG-mod-H2 equation (—) and the SGERG-88 equation (---) from the GERG-2008 equation for different natural gases ( $t = 10^\circ\text{C}$ ,  $x_{H_2} = 0\text{--}20$  mol%).



**Figure 5-4:** Relative deviations of the **SGERG-mod-H2 equation** (—) and the **SGERG-88 equation** (---) from the **GERG-2008 equation** for different natural gases and pure hydrogen ( $t = 10^\circ\text{C}$ ,  $x_{H_2} = 30\text{--}100 \text{ mol\%}$ ).

## Symbols

$\rho$	<i>density</i>
$d$	relative density
$k$	gas law deviation factor ( $=Z/Z_n$ )
$M$	molar mass
$P$	pressure
$R$	molar gas constant
$T$	temperature
$Z$	compression factor

## Indices

$n$	standard conditions
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## References

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- [12] M. Richter, M. Ben Souissi, R. Span and P. Schley, "Accurate ( $p, \rho, T, x$ ) Measurements of Hydrogen-Enriched Natural-Gas Mixtures at  $T = (273.15, 283.15, \text{ and } 293.15)$  K with Pressures up to 8 MPa," *J. Chem. Eng. Data*, vol. 29, pp. 2021-2029, 2014.
- [13] M. Jaeschke, H.-M. Hinze and A. Humphreys, Supplement to the GERG Databank of High-Accuracy Compression Factor Measurements, Düsseldorf, GERG Technical Monograph TM7.
- [14] DVGW G260, DVGW Arbeitsblatt G 260: Gasbeschaffenheit. Technische Regel, Bonn: DVGW Deutscher Verein des Gas- und Wasserfaches e. V., 2020.
- [15] AGA Transmission Measurement Committee, *Thermodynamic Properties of Natural Gas and Related Gases: DETAIL and GROSS Equations of State. AGA Report No. 8, Part I, 3rd ed., Catalog No. XQ1704-1*, 2017.



## Annexes

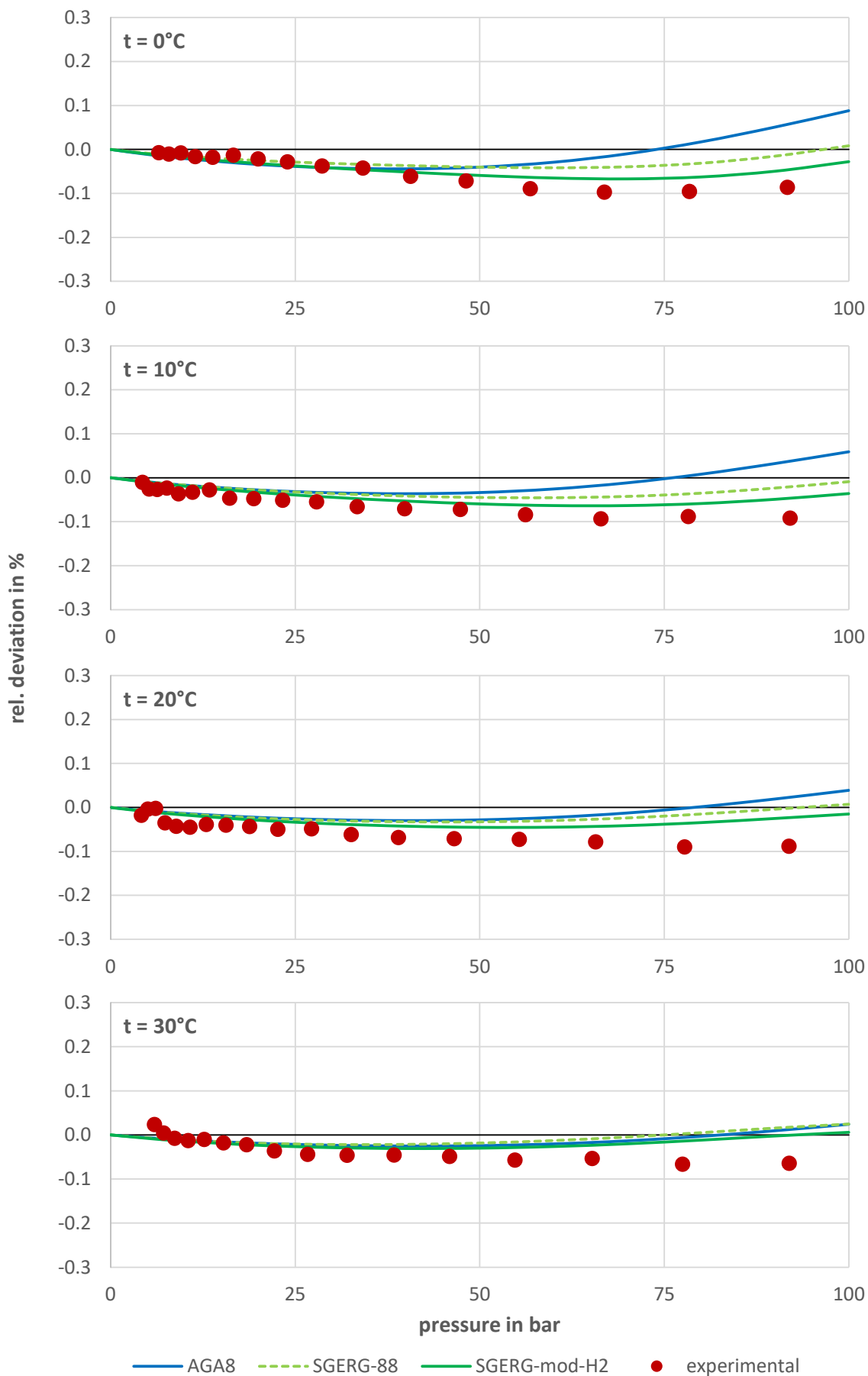
**Annex A:** Comparison for natural Gases (GERG data base TM7)

**Annex B:** Comparison for binary mixtures (GERG data base TM7)

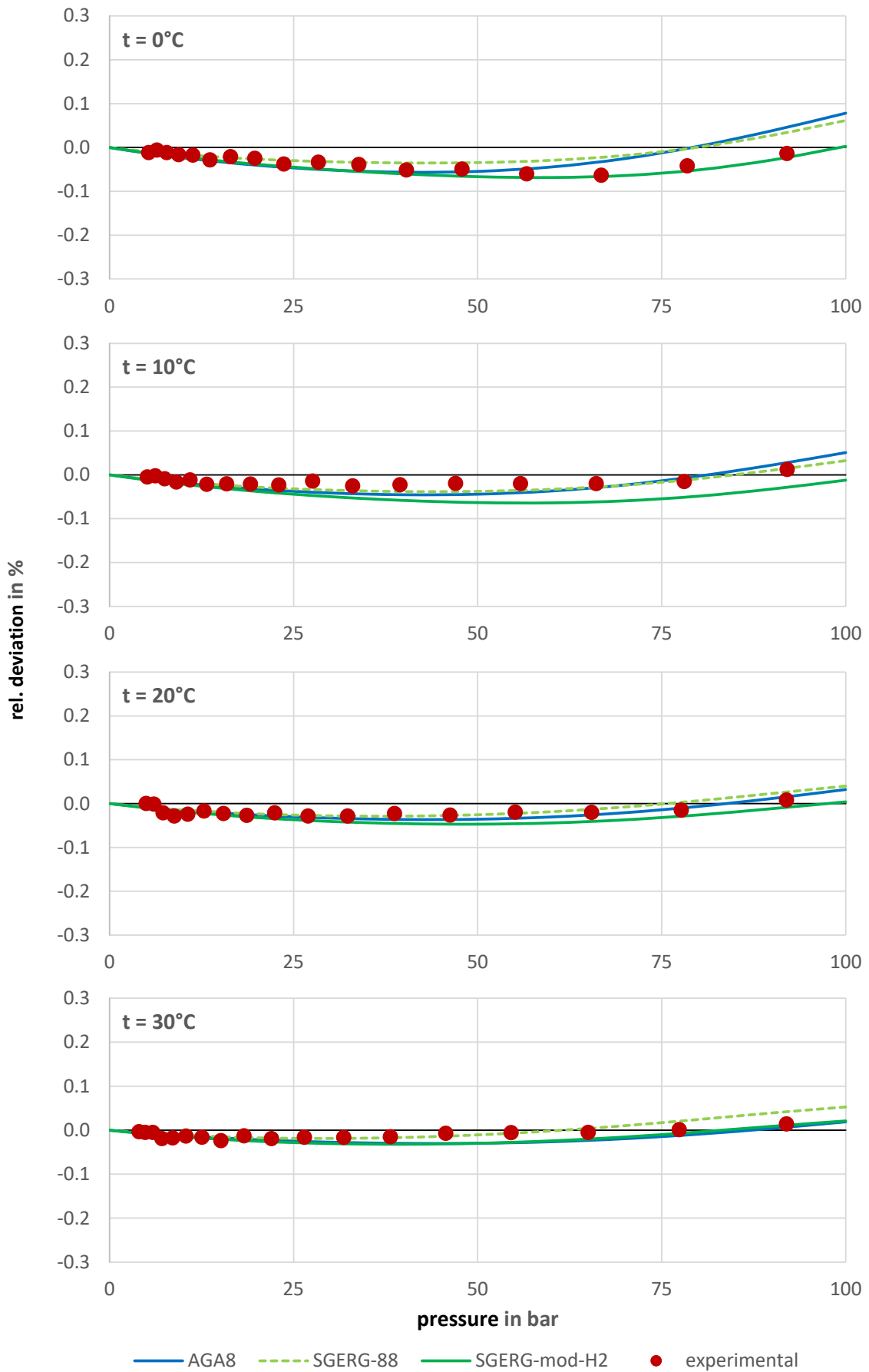
**Annex C:** Gas composition of natural gases of the experimental data sets

**Annex D:** Gas composition of natural gases from the DVGW code G260 for the comparison between the different equations of state

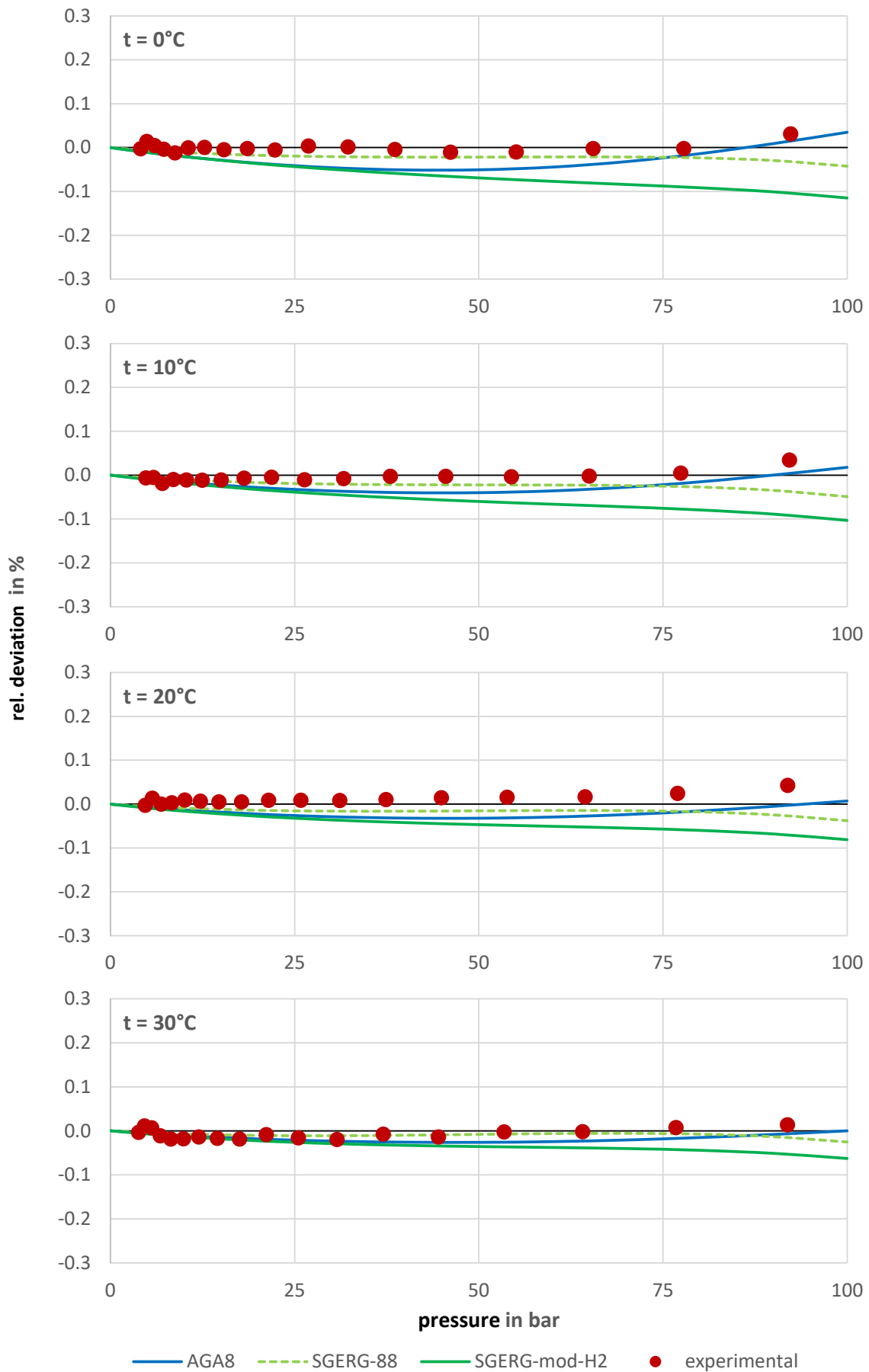
**Annex E:** Modifications of the SGERG-mod-H2 (Fortran Source Code ISO12213-3)



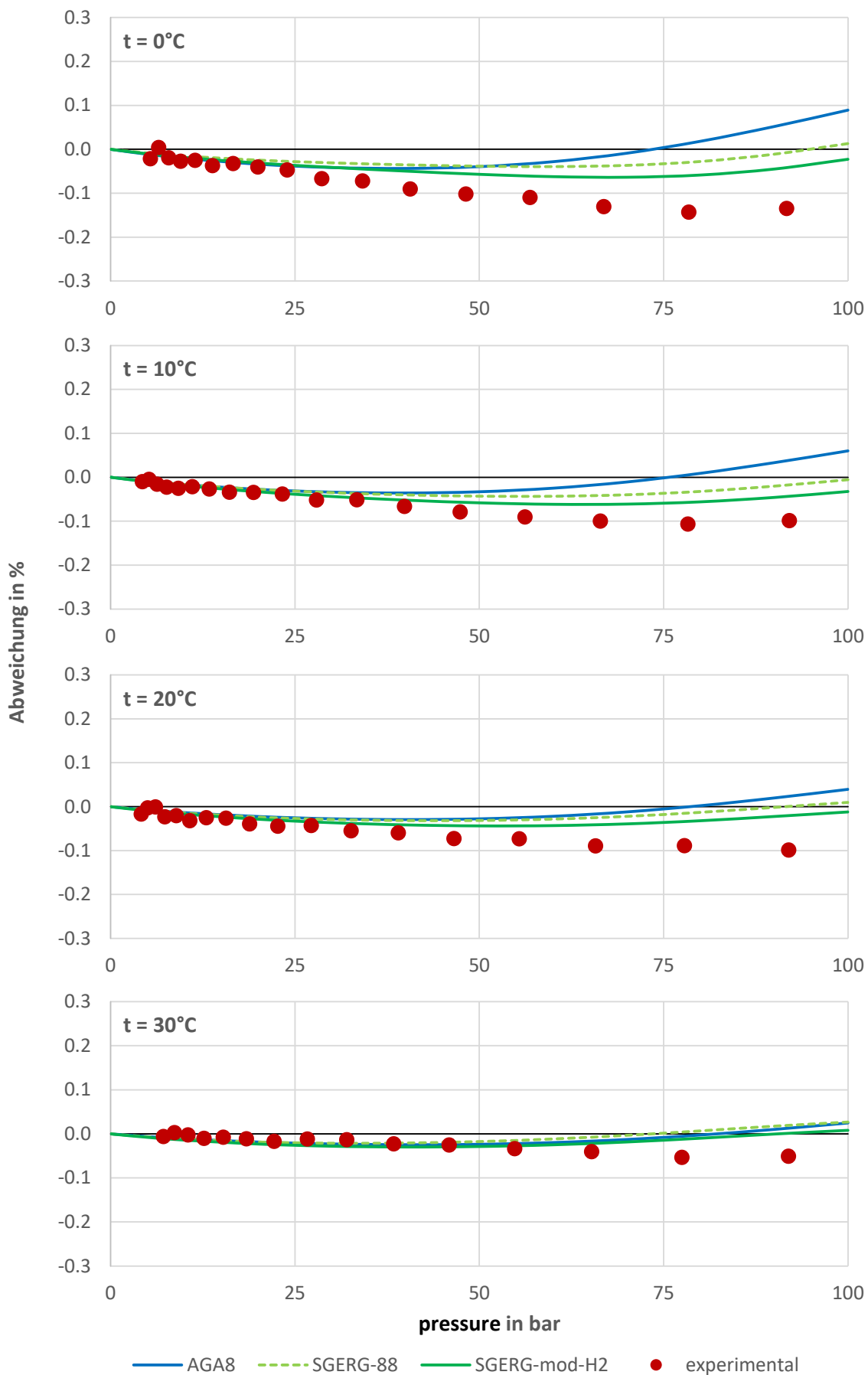
**Annex A1:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **N67** ( $x_{H_2} = 2,3094$  mol%).



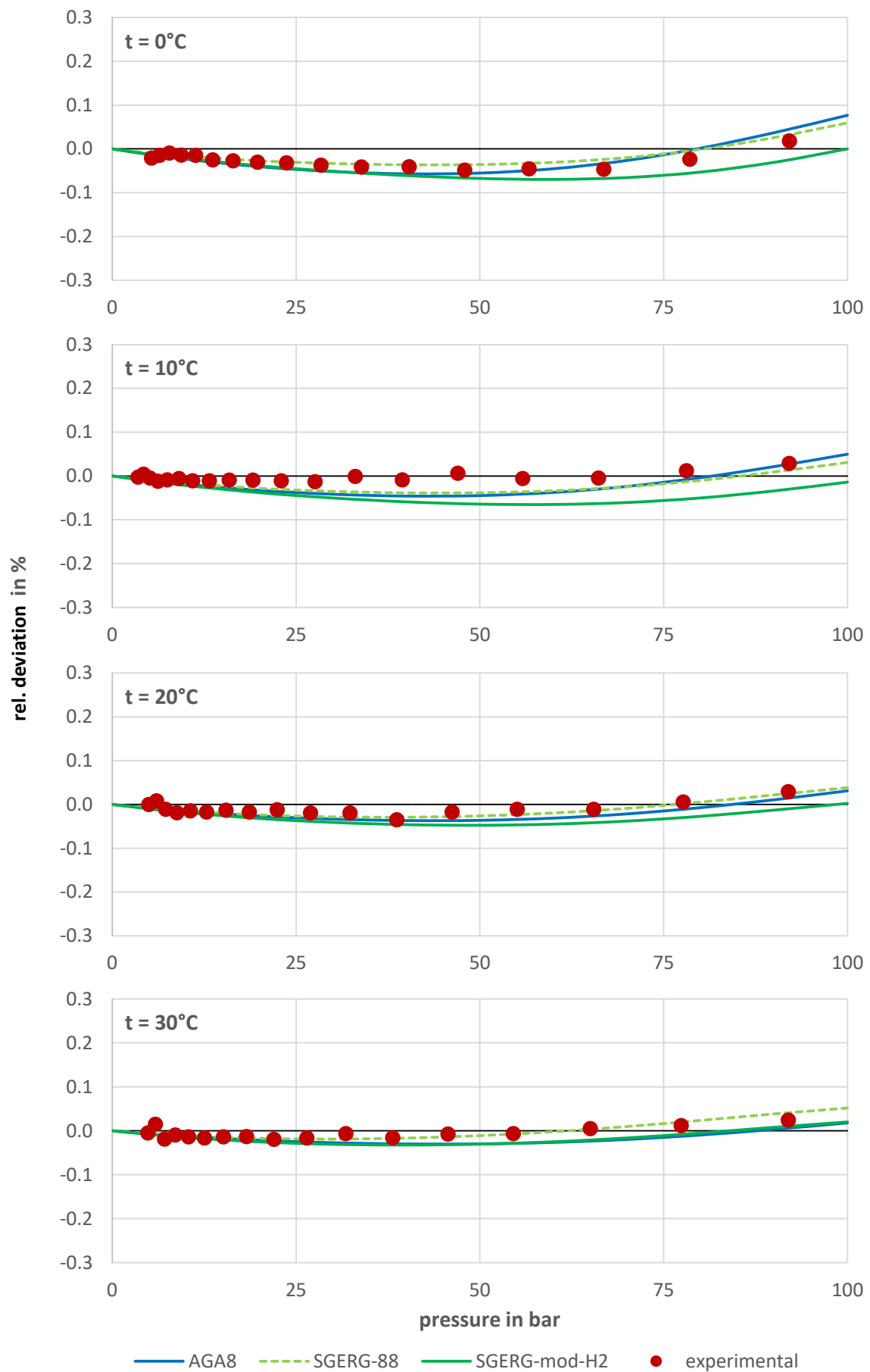
**Annex A2:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **N68** ( $x_{H_2} = 4,1947$  mol%).



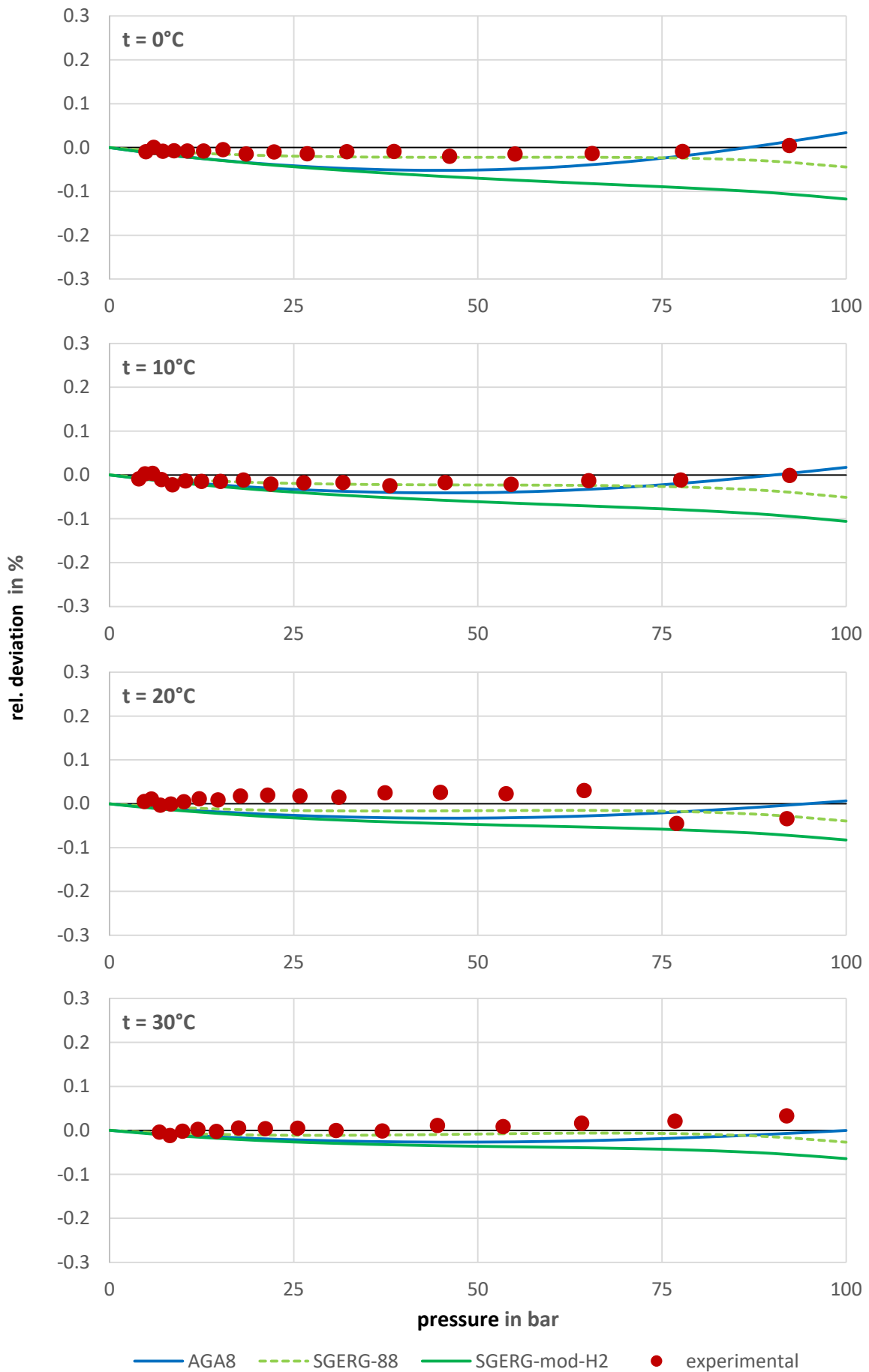
**Annex A3:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **N69** ( $x_{\text{H}_2} = 9,3919$  mol%).



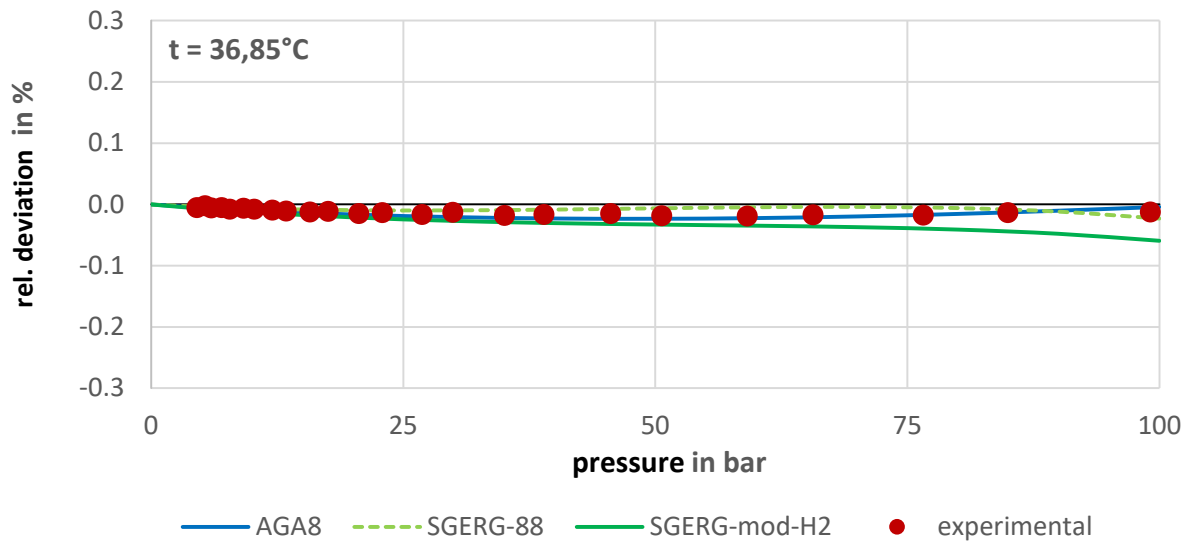
**Annex A4:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **N70** ( $x_{\text{H}_2} = 2,2770 \text{ mol}\%$ ).



**Annex A5:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **N71** ( $x_{H_2} = 4,2203$  mol%).

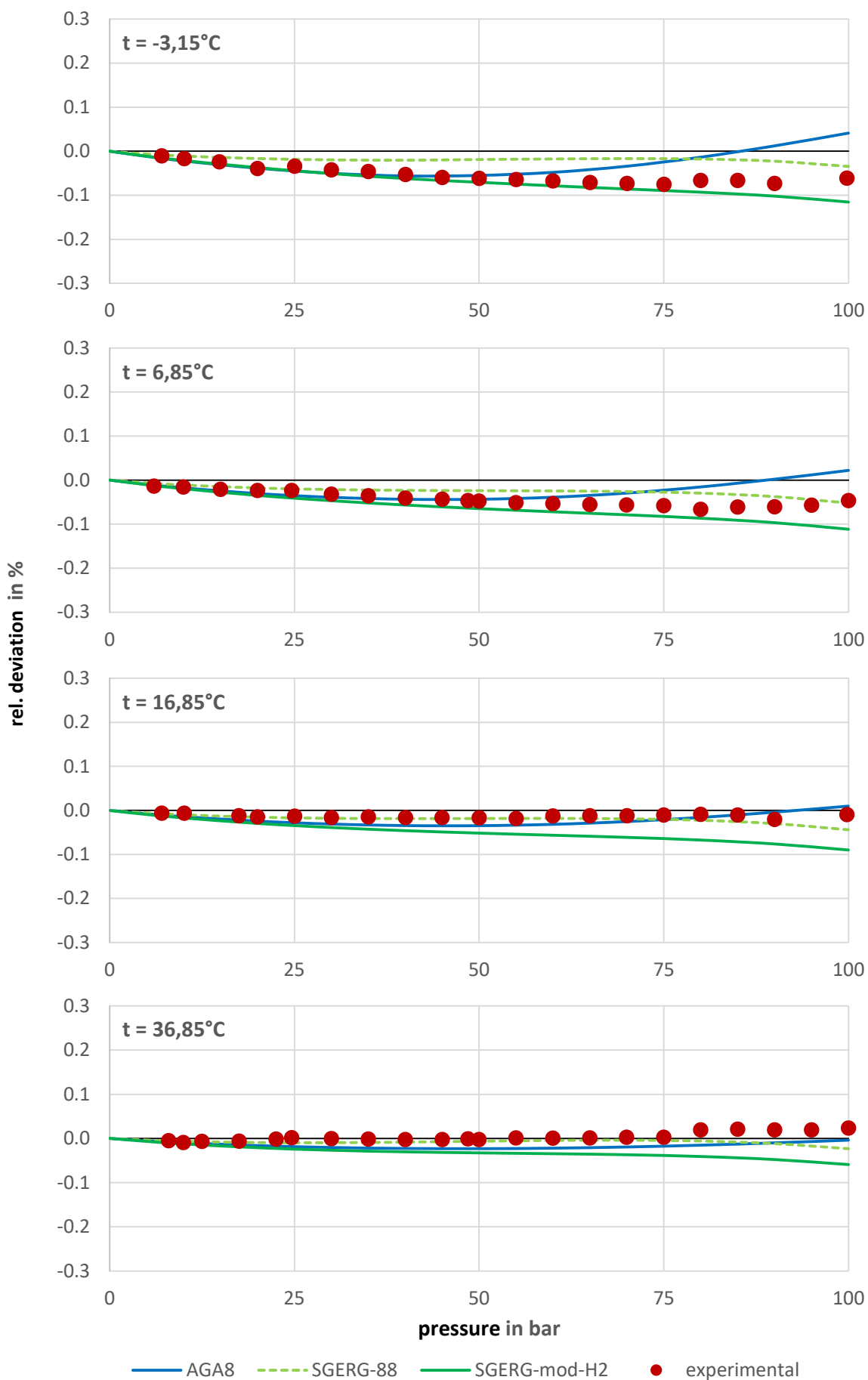


**Annex A6:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **N72** ( $x_{H_2} = 9,4918$  mol%).



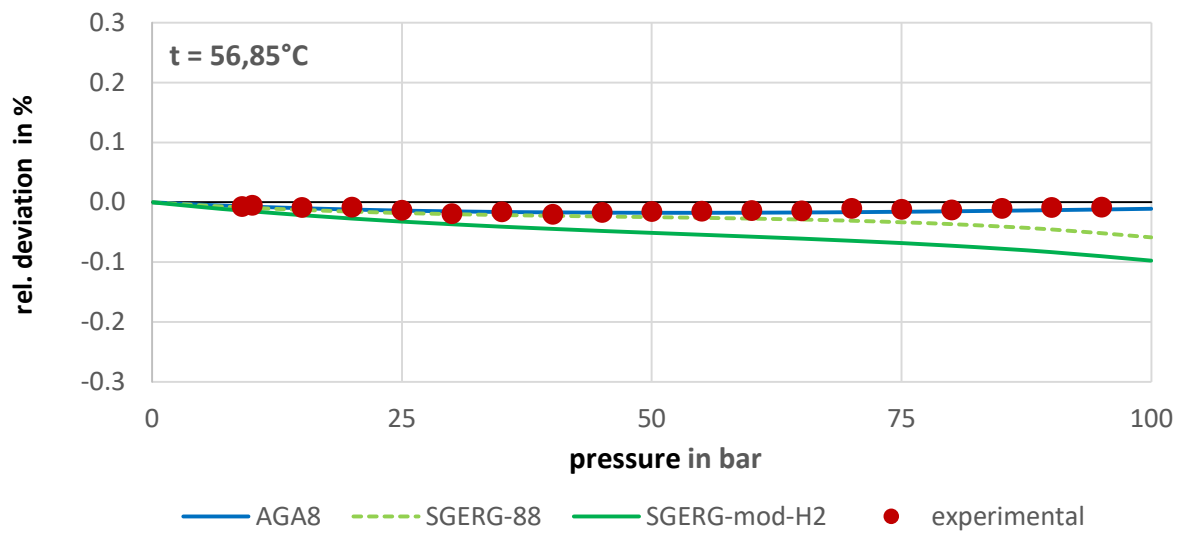
**Annex A7:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **N73** ( $x_{H_2} = 9,4918$  mol%).



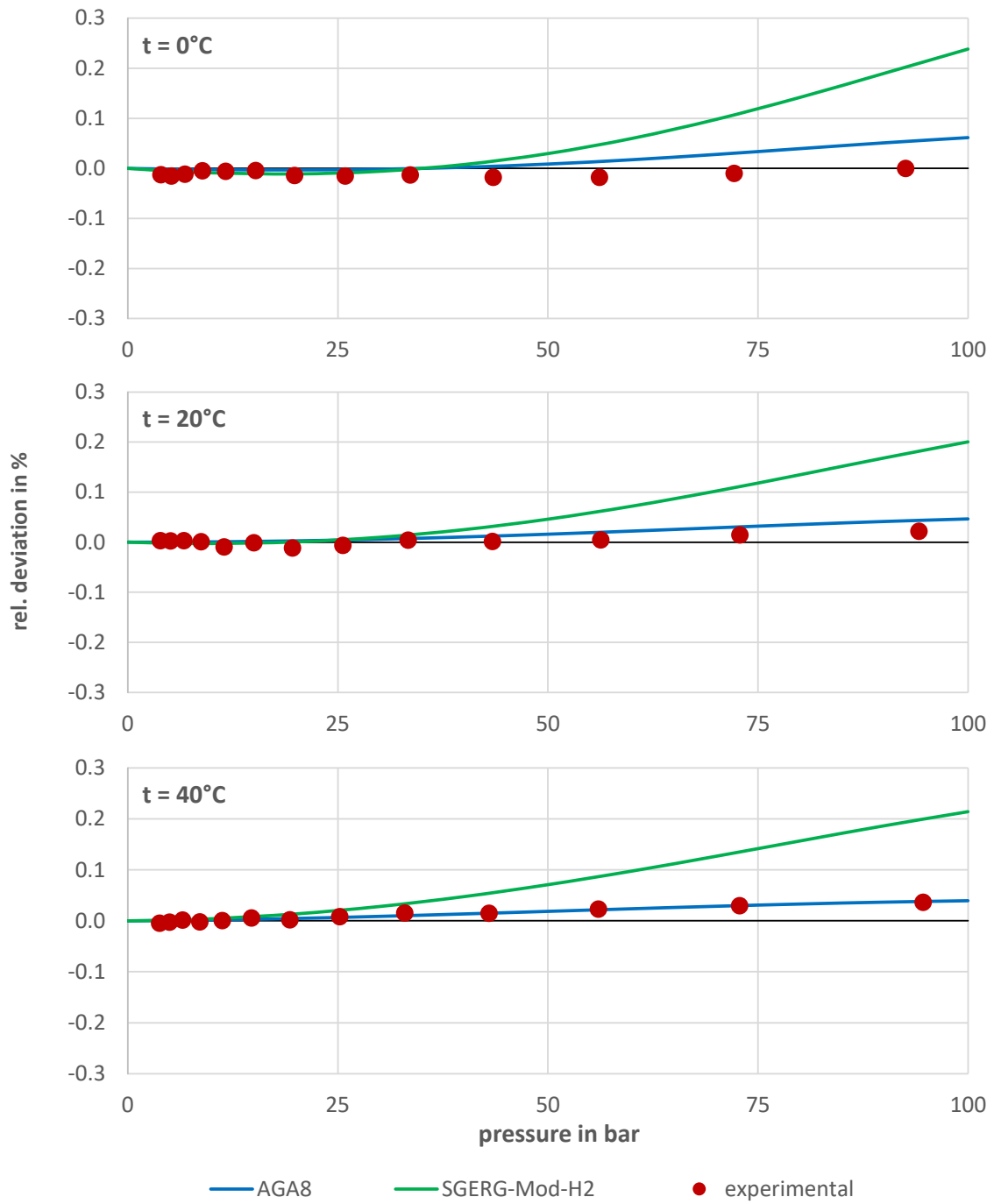


**Annex A8:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **N74** ( $x_{H_2} = 9,4918$  mol%).

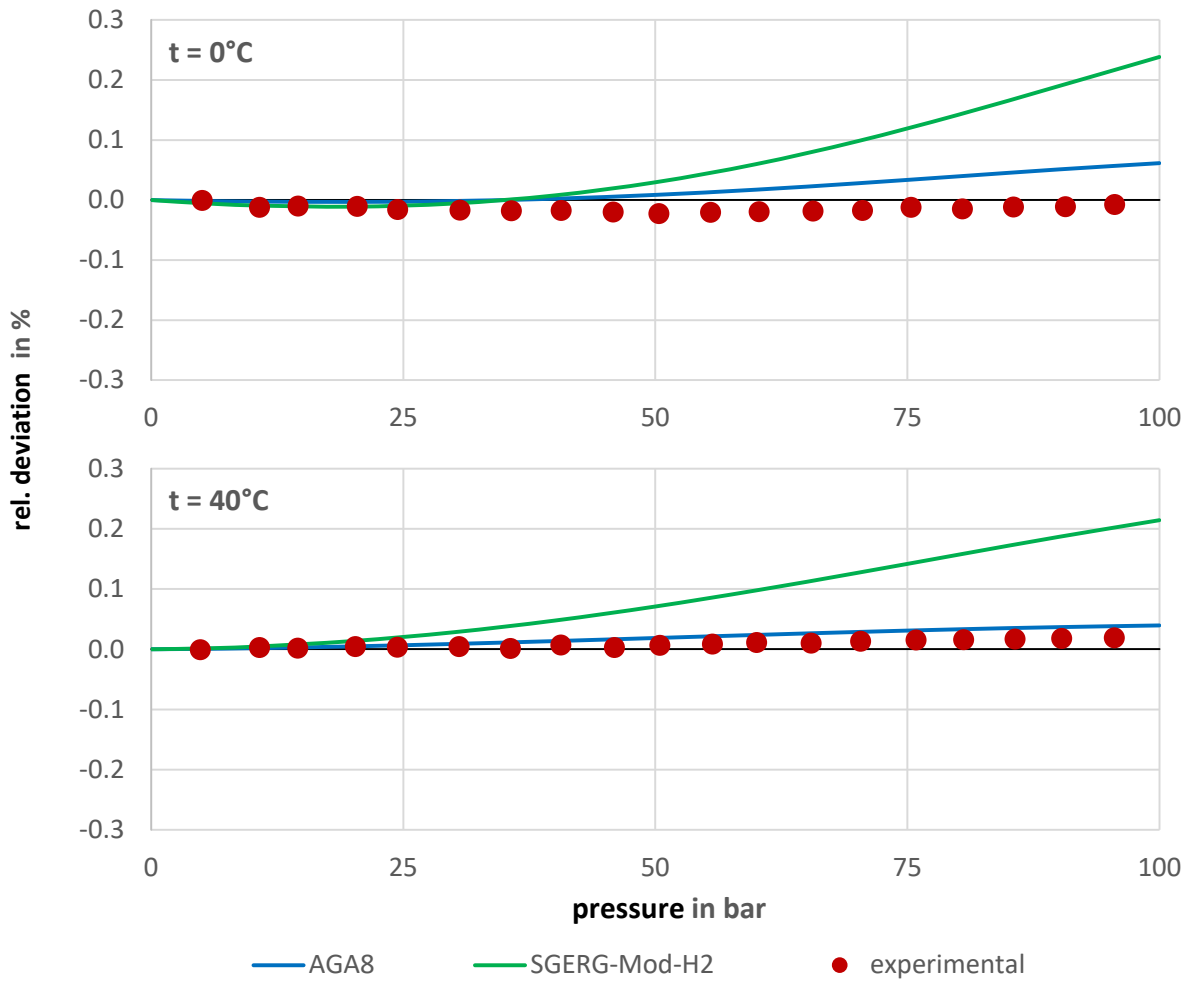
## Annex A8 (continuation)



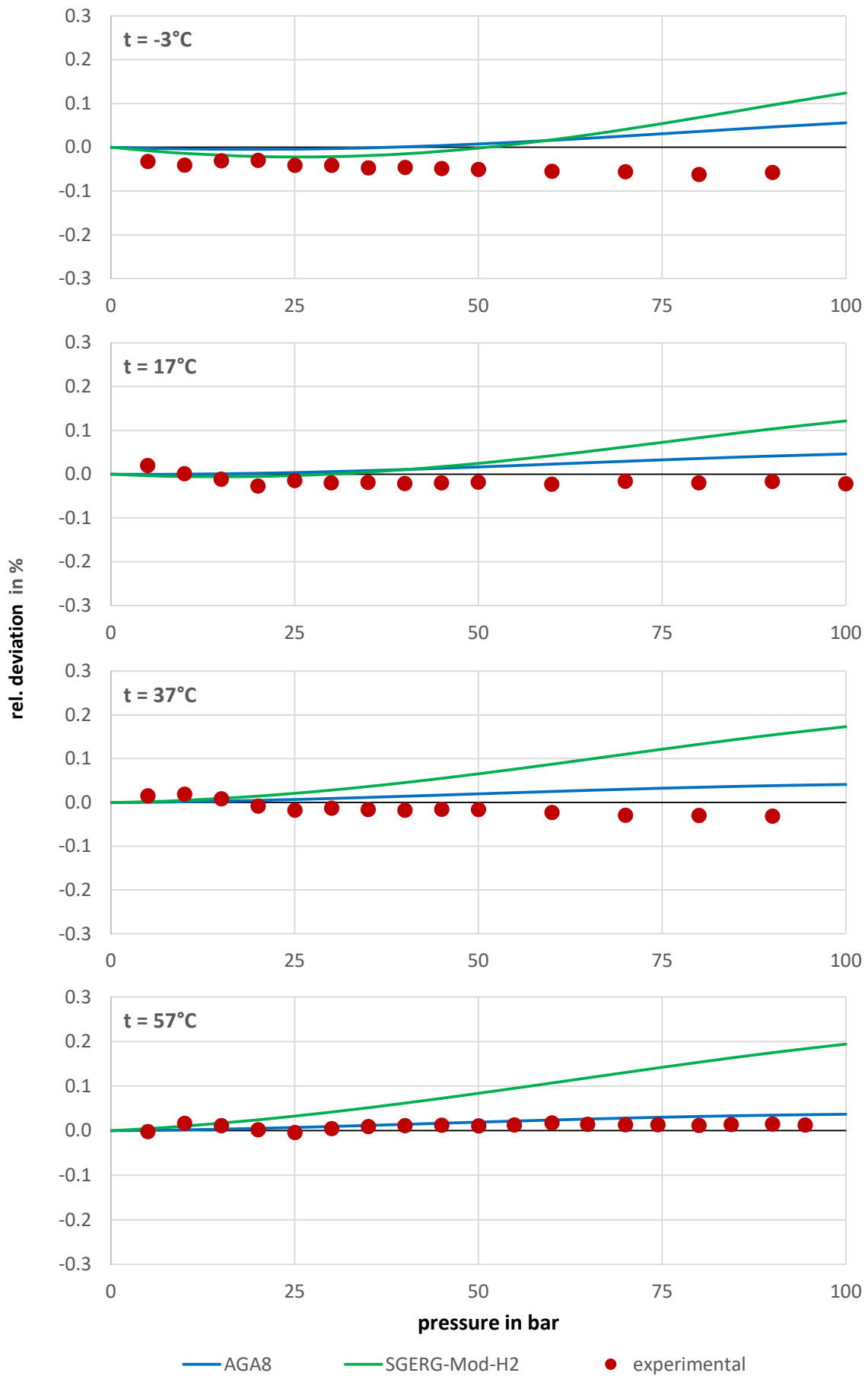
**Annex A8:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **N74** ( $x_{\text{H}_2} = 9,4918 \text{ mol}\%$ ).



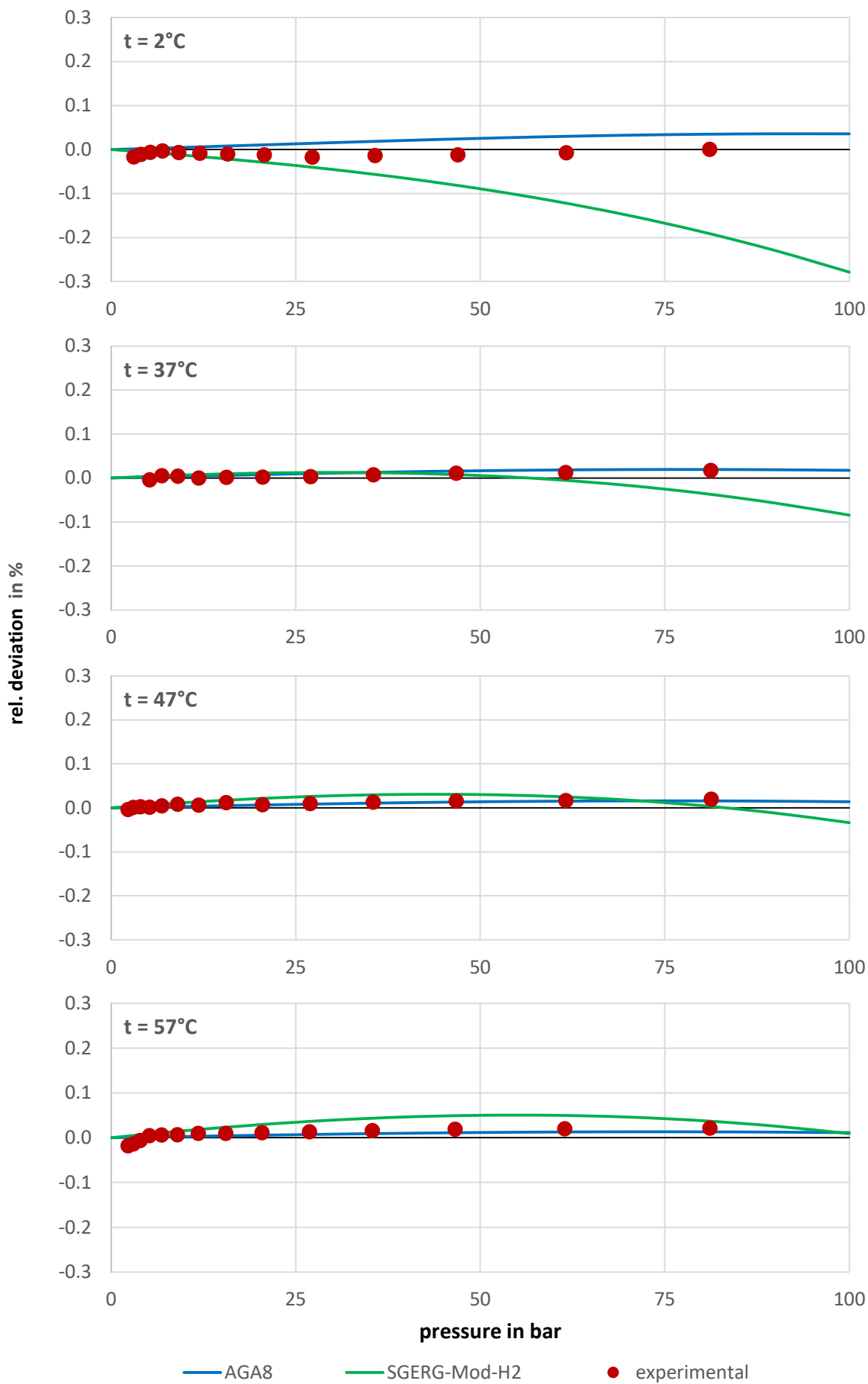
**Annex B1:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **B1** ( $x_{\text{H}_2} = 15,020 \text{ mol\%}$ ).



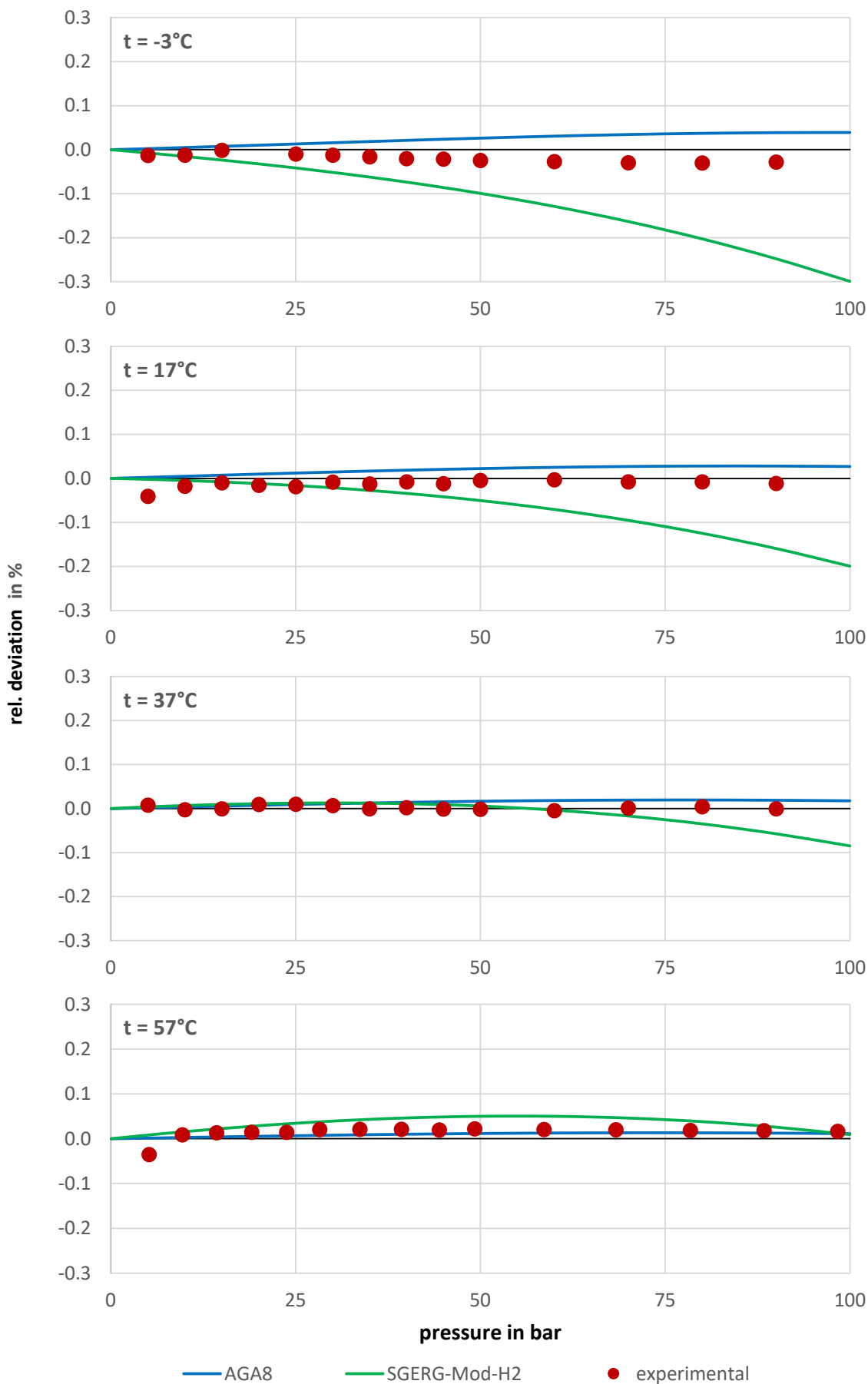
**Annex B2:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **B2** ( $x_{\text{H}_2} = 15,020 \text{ mol\%}$ ).



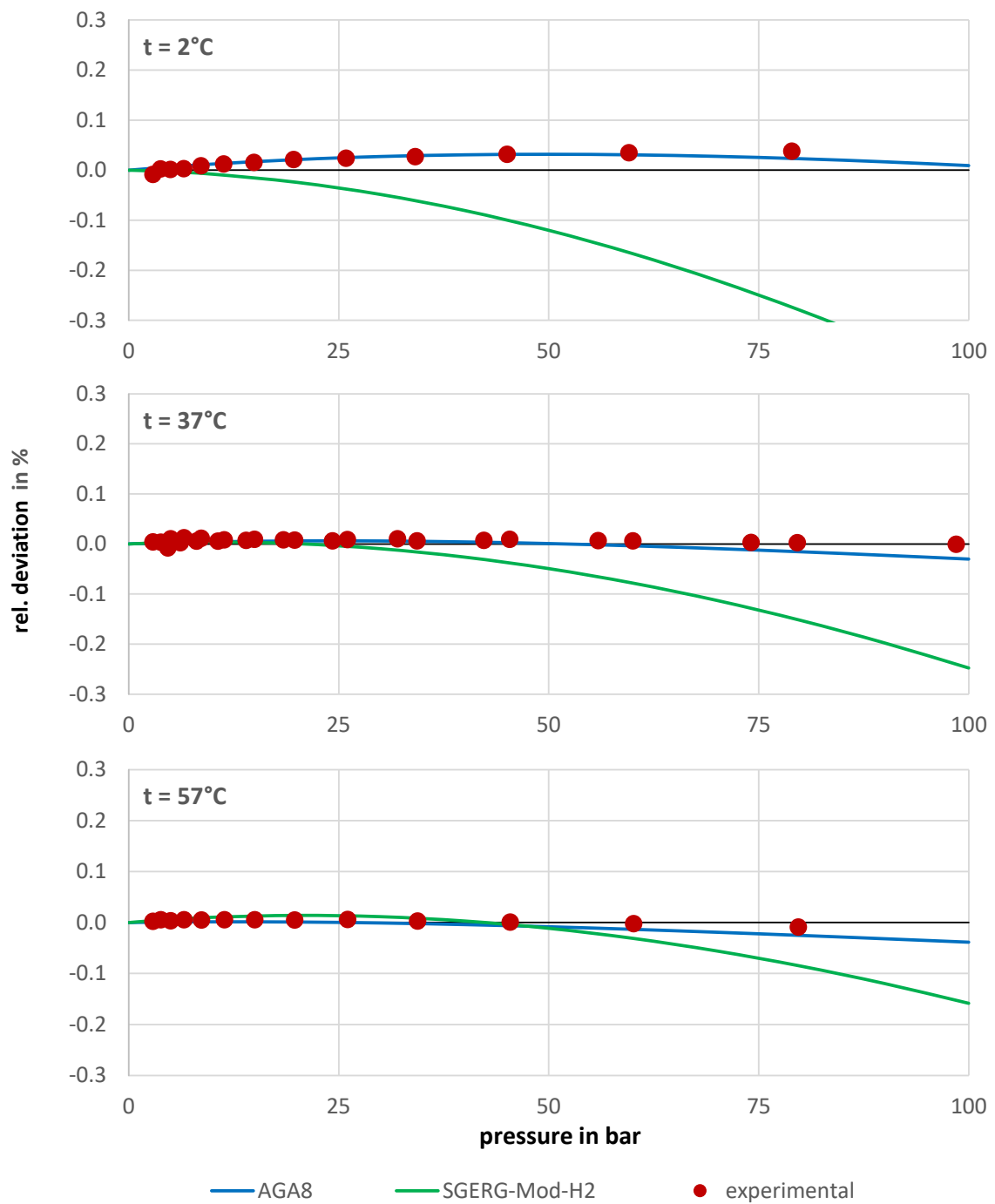
**Annex B3:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **B3** ( $x_{\text{H}_2} = 25,309$  mol%).



**Annex B4:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **B4** ( $x_{H_2} = 50,266$  mol%).

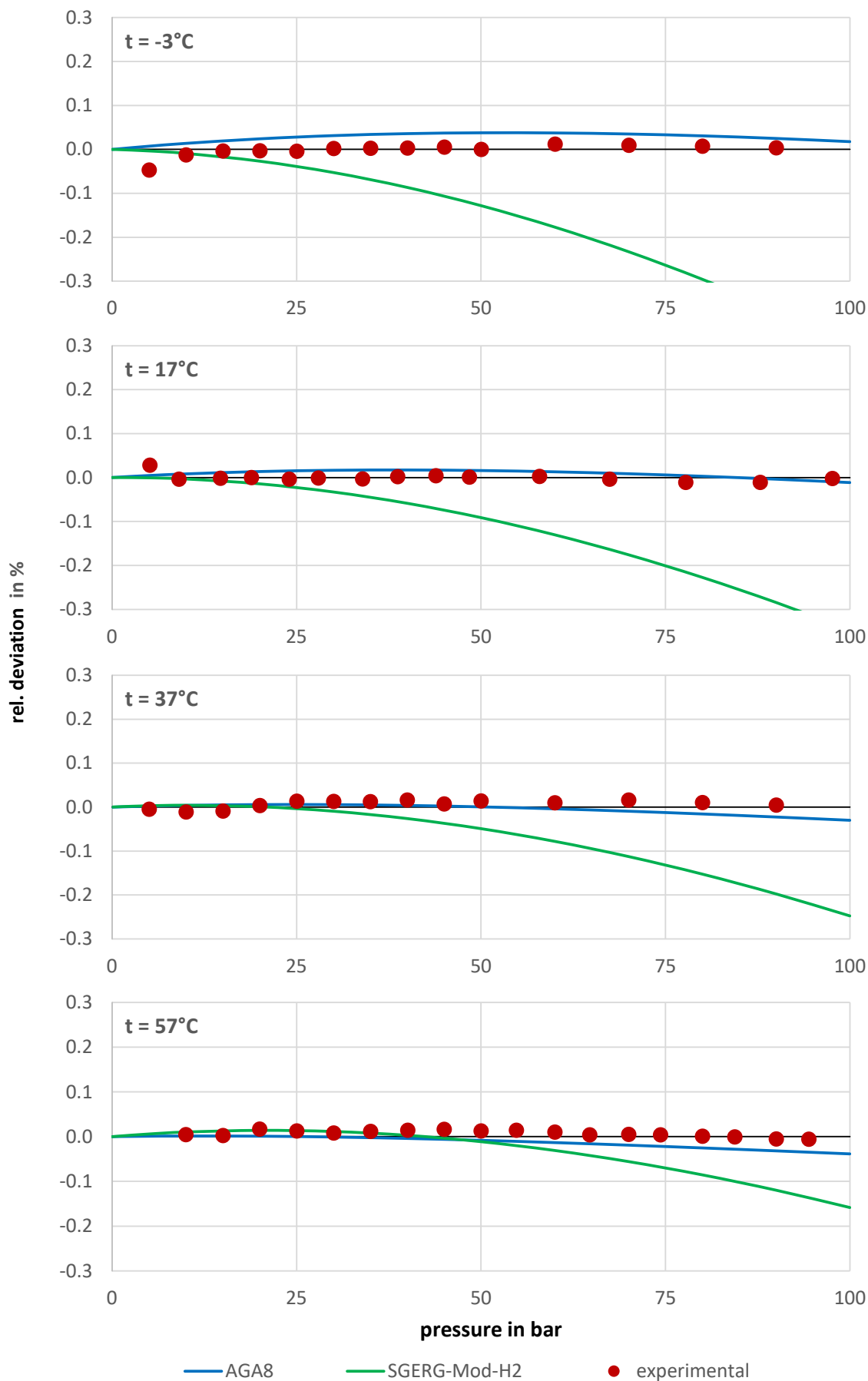


**Annex B5:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **B5** ( $x_{\text{H}_2} = 50,266$  mol%).



**Annex B6:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **B6** ( $x_{\text{H}_2} = 74,940 \text{ mol\%}$ ).





**Annex B7:** Deviations of experimental and calculated compression factors from the GERG-2008 equation for data set **B7** ( $x_{\text{H}_2} = 74,940 \text{ mol\%}$ ).



**Annex D:** Gas composition of natural gases from the DVGW code G260 for the comparison between the different equations of state.

Gas component	Symbol	Russia H	North sea H	Denmark H	Netherlands L	Germany L
Methane	$x_i(\text{CH}_4)$	96,96	88,71	90,07	83,64	86,46
Nitrogen	$x_i(\text{N}_2)$	0,86	0,82	0,28	10,21	10,24
Carbon dioxide	$x_i(\text{CO}_2)$	0,18	1,94	0,60	1,68	2,08
Ethane	$x_i(\text{C}_2\text{H}_6)$	1,37	6,93	5,68	3,56	1,06
Propane	$x_i(\text{C}_3\text{H}_8)$	0,45	1,25	2,19	0,61	0,11
n-Butane	$x_i(\text{n-C}_4\text{H}_{10})$	0,15	0,28	0,90	0,19	0,03
2-Methylpropane	$x_i(\text{i-C}_4\text{H}_{10})$					
n-Pentane	$x_i(\text{n-C}_5\text{H}_{12})$	0,02	0,05	0,22	0,04	0,01
2-Methylbutane	$x_i(\text{i-C}_5\text{H}_{12})$					
n-Hexane	$x_i(\text{n-C}_6\text{H}_{14})$	0,01	0,02	0,06	0,07	0,01
n-Heptane	$x_i(\text{n-C}_7\text{H}_{16})$					
n-Octane	$x_i(\text{n-C}_8\text{H}_{18})$					
n-Nonane	$x_i(\text{n-C}_9\text{H}_{20})$					
n-Decane	$x_i(\text{n-C}_{10}\text{H}_{22})$					
Helium	$x_i(\text{He})$					
Argon	$x_i(\text{Ar})$					
Hydrogen	$x_i(\text{H}_2)$					
Oxygen	$x_i(\text{O}_2)$					
Carbon monoxide	$x_i(\text{CO})$					
Water	$x_i(\text{H}_2\text{O})$					
Hydrogen sulfide	$x_i(\text{H}_2\text{S})$					
<b>Total</b>		<b>100,00</b>	<b>100,00</b>	<b>100,00</b>	<b>100,00</b>	<b>100,00</b>

**Annex E: Modifications of the SGERG-mod-H2 (Fortran Source Code ISO12213-3)**

```

C   SYNTAX :   CALL SGERG(X2,X3,HS,RM,X5,P,TC,Z,D)
C
C   The coefficients used in this program are conform with the
C   values of subroutine GAS682, from July 20,1988, appended to
C   report 8807, Van der Waals Laboratory, Amsterdam.
C
C   J.P.J. Michels   &   J.A. Schouten
C   August 16, 1991
C
C   Values for the gas constant, molar masses, calorific values
C   and the density of air are conform with ISO/DIS 6976 (1991).
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
SUBROUTINE SGERG(X2,X3,HS,RM,X5,P,TC,Z,D)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
IF( P.LT. 0.0 .OR. P .GT.120.0) STOP ' PRESSURE OUT OF RANGE'
IF(TC.LT.-10.0 .OR. TC.GT .65.0) STOP ' TEMPERATURE OUT OF RANGE'
CALL SGERG1(P,TC,X2,X3,X5,HS,RM,Z,D)
RETURN
END
C
*****
SUBROUTINE SGERG1(P,TC,Q2,Q3,Q5,QM,RM,Z,D)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
COMMON /RBLOK/ AMOL,HS
COMMON /XBLOK/ X1,X2,X3,X11,X12,X13,X22,X23,X33
> ,X5,X7,X15,X17,X25,X55,X77
COMMON /MBLOK/ GM1R0,GM1R1,GM2,GM3,GM5,GM7,FA,FB,RL,T0,H5,H7,R
HS = QM
X3 = Q3
X5 = Q5
IF(RM.LT. 0.55.OR. RM.GT. 0.90) STOP 'REL. MASS OUT OF RANGE'
IF(RM.LT. 0.06.OR. RM.GT. 0.90) STOP 'REL. MASS OUT OF RANGE'
IF(X3.LT. 0.0 .OR. X3.GT. 0.30) STOP 'CO2 OUT OF RANGE'
IF(HS.LT.20.0 .OR. HS.GT.48.0 ) STOP 'CALOR. VALUE OUT OF RANGE'
IF(HS.LT. 6.0 .OR. HS.GT.48.0 ) STOP 'CALOR. VALUE OUT OF RANGE'
IF((0.55+0.97*X3-0.45*X5).GT.RM)STOP 'CONFLICTING INPUT'
SM = RM*RL
X7 = X5*0.0964D0
X7 = 0D0

```

set lower limit of the relative density to „0.06“

set lower limit of the calorific value to „6 MJ/m<sup>3</sup>“

suppress consistency check for standard density

suppress CO correction

```

X33 = X3*X3
X55 = X5*X5
X77 = X7*X7
BEFF= 0.065D0
BEFF= 0D0
H = 1000.0D0
AMOL= 1.0D0/(FA+BEFF)
K = 0
KK = 0
1 CALL SMBER(H,SMT1)
  IF (ABS(SM-SMT1) .GT. 1.D-6) THEN
    CALL SMBER(H+1.0D0,SMT2)
    DH= (SM-SMT1)/(SMT2-SMT1)
    H = H+DH
    KK = KK+1
    IF (KK.GT.20) STOP 'NO CONVERGENCY #1'
    GO TO 1
  END IF
X11 = X1*X1
X12 = X1*X2
X13 = X1*X3
X22 = X2*X2
X23 = X2*X3
X25 = X2*X5
X15 = X1*X5
X17 = X1*X7
CALL B11BER(T0,H,B11)
CALL BBER(T0,B11,BEFF)
AMOL= 1.0D0/(FA+BEFF)
HSBER = X1*H*AMOL+(X5*H5+X7*H7)*AMOL
IF (ABS(HS-HSBER) .GT.1.0D-4) THEN
  K = K+1
  IF (K.GT.20) STOP 'NO CONVERGENCY #2'
  GO TO 1
END IF
IF (X2.GT.0.5) STOP 'CALC. N2 OUT OF RANGE'
IF (X2+X3.GT.0.5) STOP 'N2 + CO2 OUT OF RANGE'
IF (X2.LT.-0.01 .OR. (0.55+.4*X2+0.97*X3-0.45*X5) .GT.PM)
+ STOP 'CONFLICTING RESULT FOR N2'
+ IF (X2.LT.-0.01)
+ STOP 'CONFLICTING RESULT FOR N2'

```

set starting value of the 2<sup>nd</sup>  
virial coefficient to „0“

suppress consistency check  
for standard density