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Measurement Science and Standards

Monte Carlo Investigation of Refractive Index Gas Thermometry Uncertainties

ABSTRACT

Refractive Index Gas Thermometry (RIGT) is a primary thermometry technique whereby the thermodynamic temperature of a working gas is determined via measurements of the refractive index of the gas. Monte Carlo calculations are presented for a microwave resonance-based RIGT arrangement under development at NRC, employing a quasi-spherical copper resonator and helium as the working gas.

Results indicate that RIGT could be a useful primary thermometry technique to supplement Acoustic Gas Thermometry (AGT) and Dielectric Constant Gas Thermometry (DCGT) thermodynamic temperature measurements between 25 K and 150 K.

Figure 1. Quasi-spherical microwave resonator & gas pressure vessel

From Rourke (2014) [1]

INTRODUCTION

- Consultative Committee for Thermometry Working Group 4 (WG4) published consensus estimate of ITS-90 temperature deviation from thermodynamic temperature – Fischer (2011) [2]
- 24.5 K – 77 K region: special interest
  - Gap in AGT results of Pitre (2006) [3]
  - Disagreement between AGT results of Pitre (2006) [3] and DCGT results of Gaiser (2010) [4]
- RIGT: similarities to both AGT & DCGT ⇒ tie-breaker?
- RIGT uncertainties: low enough to contribute meaningfully to $T - T_{90}$?
  - Treated at 1 standard deviation level in present work

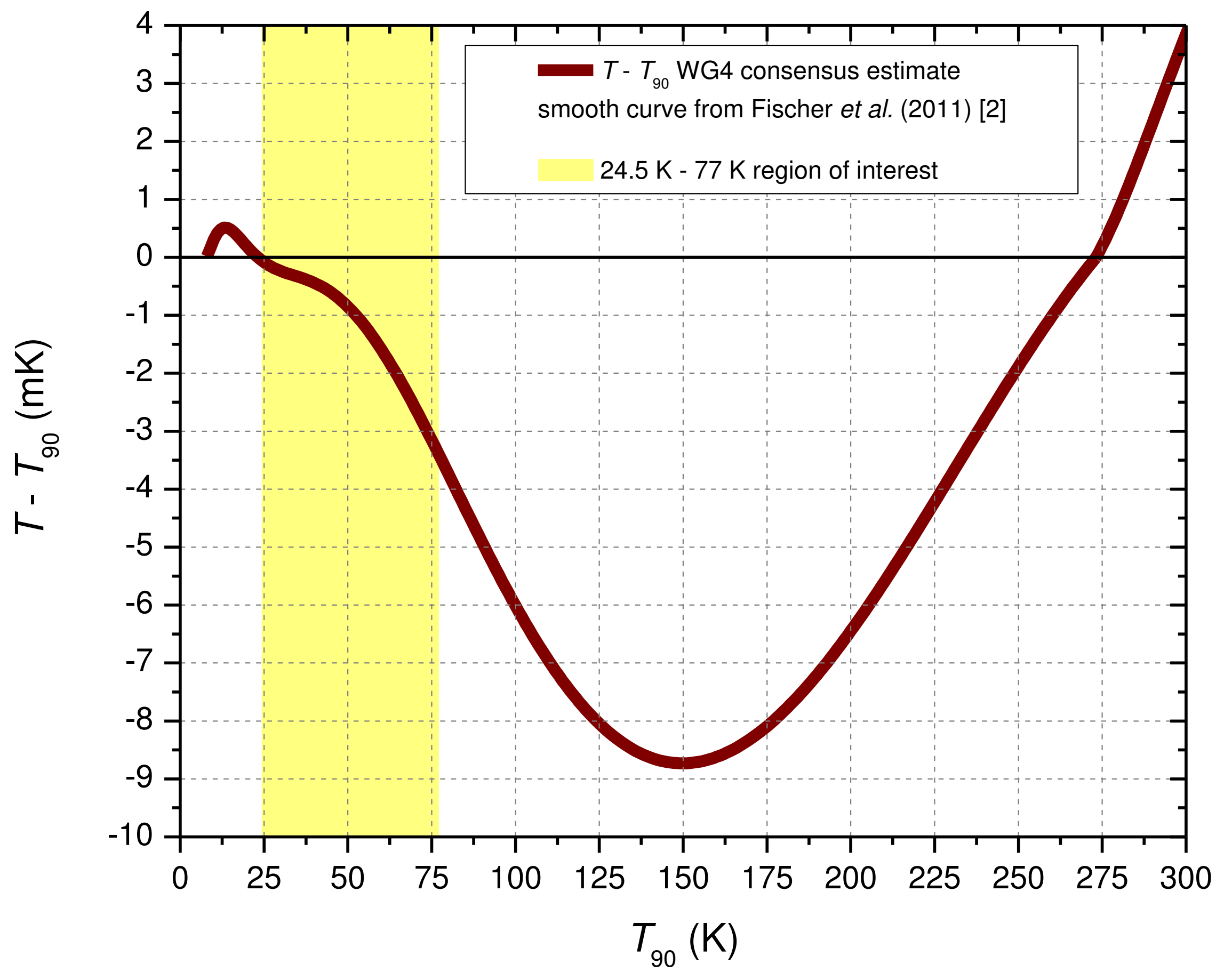

Figure 2. Consensus estimate of ITS-90 temperature T_{90} deviation from thermodynamic temperature T

From Fischer (2011) [2]

MAIN EQUATIONS

- Gas refractive index n_{expt} obtained experimentally, in which c_0 is the speed of light in vacuum and $<\xi_{\mathrm{corr}}>$ is the average corrected microwave eigenvalue, as per Rourke (2014) [1]

$$n_{\mathrm{expt}}^2 - 1 = \left\{ \frac{c_0}{2\pi \cdot \langle f+g \rangle (T)} \cdot \frac{\langle \xi_{\mathrm{corr}} \rangle}{a_0(T) \cdot \left[1 - \frac{\kappa_{\mathrm{T}}(T) \cdot p}{3} \right]} \right\}^2 - 1$$

- Copper isothermal compressibility κ_{T}

$$\kappa_{\mathrm{T}} = \frac{1}{B_{\mathrm{S}}} + \frac{9 \cdot \alpha_{\mathrm{L}}^2(T) \cdot T \cdot a_0^3(T)}{\rho_{\mathrm{Cu}}(T = 293\ \mathrm{K}) \cdot c_{\mathrm{p}}(T) \cdot a_0^3\ (T = 293\ \mathrm{K})}$$

- Gas pressure p virial equation in terms of the molar gas density ρ

$$p \approx RT \cdot \left[\rho + B_\rho(T) \cdot \rho^2 + C_\rho(T) \cdot \rho^3 + D_\rho(T) \cdot \rho^4 \right]$$

- Gas pressure virial equation inverted by iterative substitution, as per Moldover (1998) [5], to get the molar gas density ρ in terms of the gas pressure p

$$\rho \approx p \Big/ \left\{ RT + \frac{B_\rho(T) \cdot p}{\left[1 + \frac{B_\rho(T) \cdot p}{RT + B_\rho(T) \cdot p} + \frac{C_\rho(T) \cdot p^2}{RT\left(RT + 2B_\rho(T) \cdot p\right)} \right]} + \frac{C_\rho(T) \cdot p^2}{RT + 2B_\rho(T) \cdot p} + \frac{D_\rho(T) \cdot p^3}{R^2 T^2} \right\}$$

- Gas relative magnetic permeability μ_{r} virial equation

$$(\mu_{\mathrm{r}} - 1)/(\mu_{\mathrm{r}} + 2) \approx A_\mu \rho$$

- Gas relative dielectric permittivity ε_{r} virial equation

$$(\varepsilon_{\mathrm{r}} - 1)/(\varepsilon_{\mathrm{r}} + 2) \approx A_\varepsilon \rho + B_\varepsilon(T) \cdot \rho^2 + C_\varepsilon \rho^3$$

- Gas refractive index n_{calc} obtained theoretically

$$n_{\mathrm{calc}}^2 - 1 = (\mu_{\mathrm{r}} \varepsilon_{\mathrm{r}}) - 1$$

PARAMETER VALUES AND UNCERTAINTIES

- Input temperature T uncertainty (temperature stability & ITS-90 realization) set to 0.2 mK
- Pressure p uncertainties from NRC's CMCs (k = 1)
  - 5 kPa – 350 kPa: 1.00 × 10^{-5} relative uncertainty
  - 350 kPa – 1750 kPa: 1.80 × 10^{-5} relative uncertainty
  - 1750 kPa – 7000 kPa: 2.50 × 10^{-5} relative uncertainty
- Average half-width-corrected microwave frequency $<f + g>$ uncertainty and resonator vacuum radius $a_0(T)$ values & uncertainties from cubic spline interpolation of Rourke (2014) [1] experimental measurements
- OFHC copper material parameters contributing to the resonator isothermal compressibility κ_{T}: adiabatic bulk modulus B_{s}, linear thermal expansion coefficient α_{L}, specific heat at constant pressure c_{p}, and density at 293 K $\rho_{\mathrm{Cu}}(T = 293\ \mathrm{K})$ – values & uncertainties from Simon (1992) [6]
  - κ_{T} uncertainty dominated by uncertainty in B_{s}
- Molar gas constant R = 8.3144621(75) J mol^{-1} K^{-1} from CODATA (2010)
- Helium gas density virial coefficients $B_\rho(T)$, $C_\rho(T)$, $D_\rho(T)$ values & uncertainties from cubic spline interpolation of Shaul (2012) [7]
- Helium gas diamagnetic virial coefficient $A_\mu = 4\pi\chi_0/3$ = -0.000007921(4) cm^3 mol^{-1} from Bruch (2000) [8], following treatment of Moldover (2014) [9]
- Helium gas molar polarizability in the limit of zero density A_ε = 0.51725419(10) cm^3 mol^{-1} from Lach (2004) [10], following treatment of Moldover (2014) [9]
- Helium gas dielectric virial coefficient $B_\varepsilon(T)$ from 5th-order polynomial fit Rizzo (2002) [11] calculated table values; uncertainties are quadrature combinations of 3 sources
  - Rizzo's expectation of convergence to within 0.1%
  - Digital display uncertainty for Rizzo table values printed to 4 decimal places without printed uncertainties
  - 5.4 × 10^{-5} cm^6 mol^{-2} standard deviation of 5th-order polynomial fit residuals
- Helium gas dielectric virial coefficient C_ε = -0.6(4) cm^9 mol^{-3} from averaging several experimental [12-15] and calculated [16] values at different temperatures; uncertainty from standard deviation of these values
  - Roughly T-independent, at least within published uncertainties

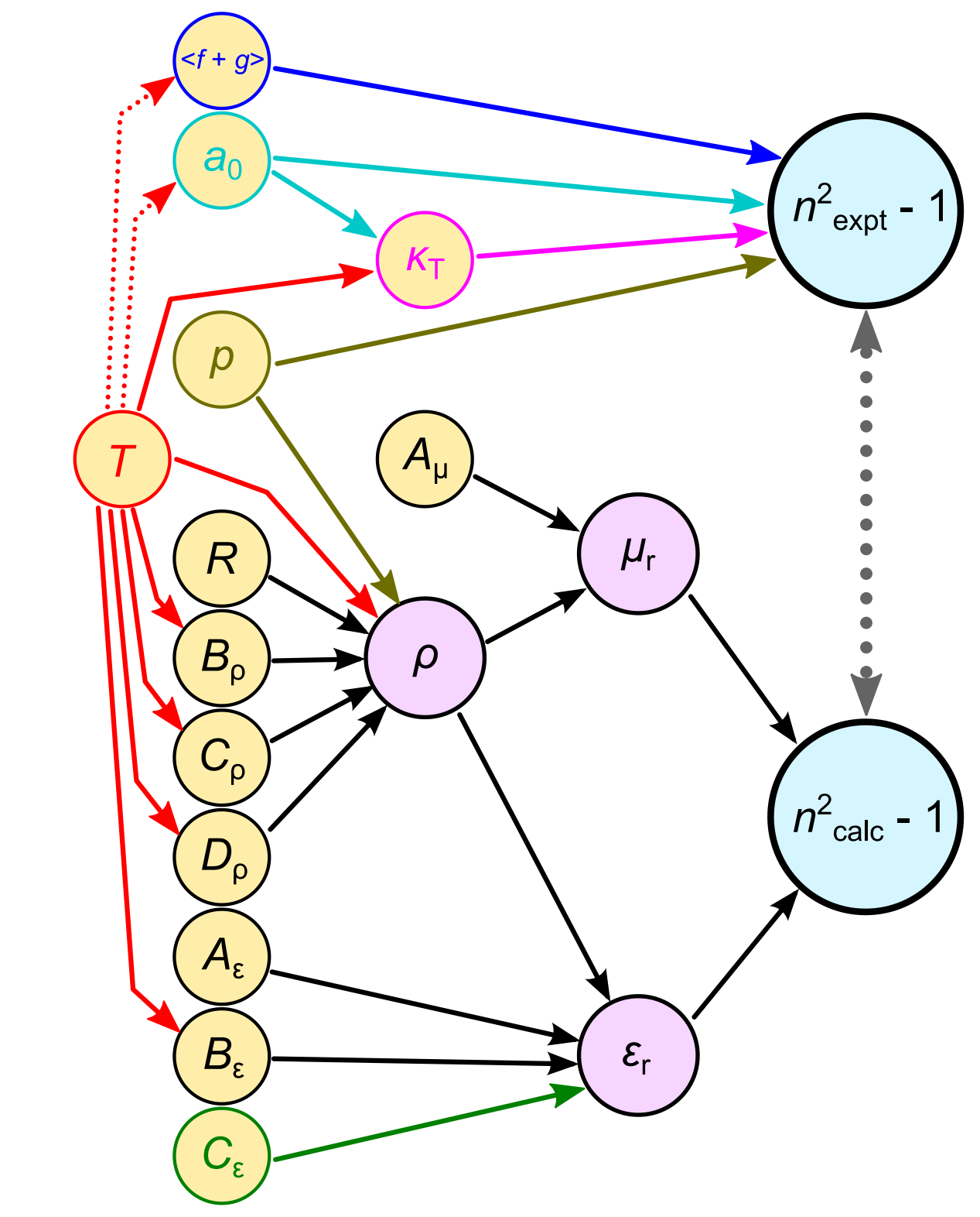

Figure 3. Relational diagram of RIGT equation parameters

Parameters with yellow backgrounds are sampled via Monte Carlo trials

MONTE CARLO CALCULATION DETAILS

For each input parameter at a given (T, p, microwave mode) point:

- Input parameter Gaussian distribution sampled 100,000 times
- Resulting $n^2 - 1$ standard deviation translated to a thermodynamic temperature T_{therm} distribution to get $\delta T_{\mathrm{therm}}$, using relationship between T distribution width and $n^2_{\mathrm{calc}} - 1$ distribution width

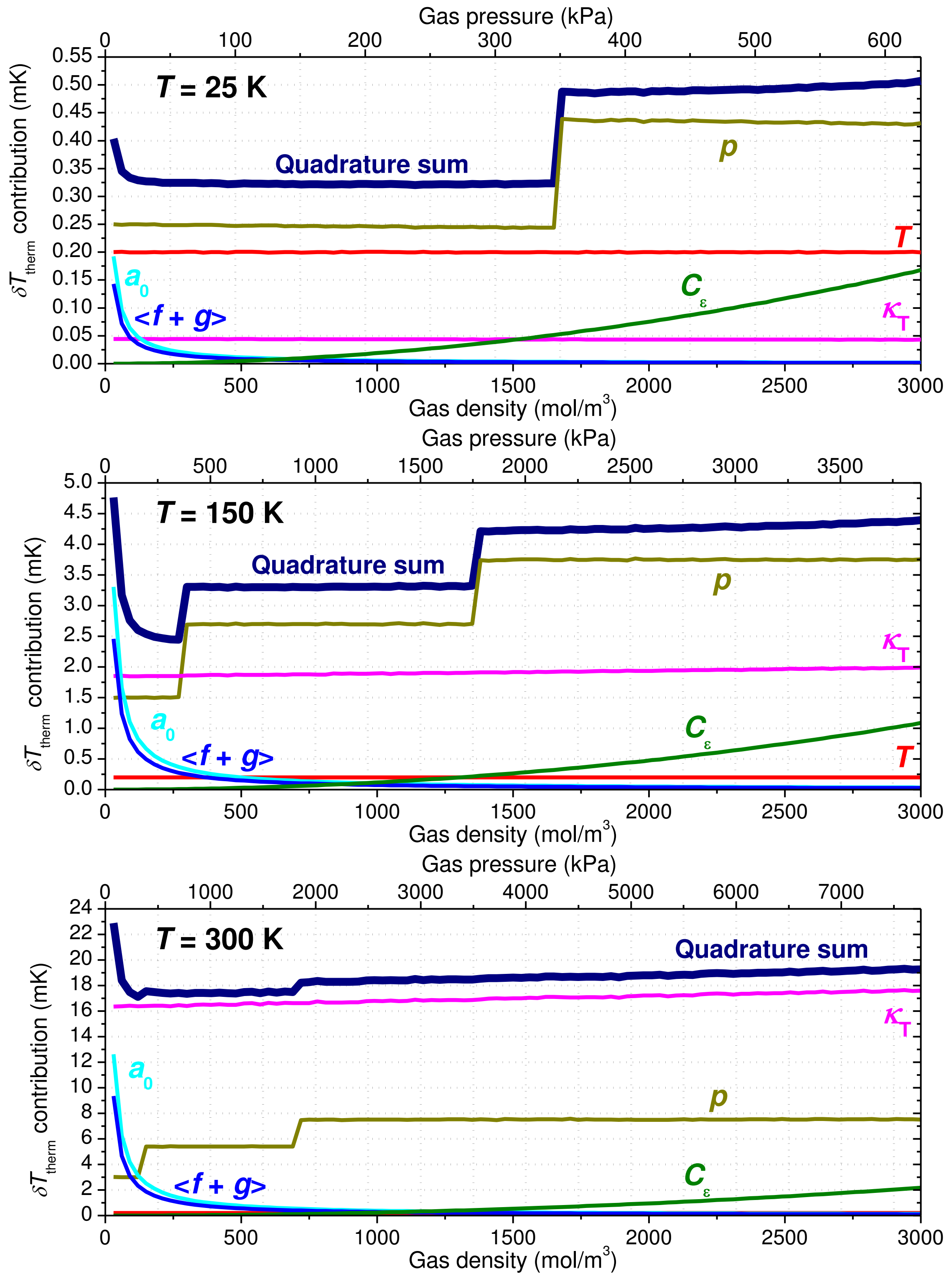

Figure 4. Dominant Monte Carlo contributions to RIGT thermodynamic temperature uncertainty

Calculated at various temperatures and gas pressures, for TM11 microwave mode

RESULTS

- RIGT thermodynamic temperature uncertainties dominated by uncertainties in gas pressure p and, at higher temperatures, resonator compressibility κ_{T}
- Best overall uncertainties obtained when $p \leq 350$ kPa
- Results for microwave modes TE11, TM12, TE12 and TM13 (not shown) similar to TM11, with increased uncertainty contributions from a_0 and $<f + g>$

Temperature T	Gas pressure p	Gas density ρ	$\delta T_{\mathrm{therm}}$ quadrature sum
25 K	350 kPa	1700 mol/m^3	0.32 mK
50 K	350 kPa	840 mol/m^3	0.57 mK
75 K	350 kPa	560 mol/m^3	0.88 mK
150 K	350 kPa	280 mol/m^3	2.4 mK
225 K	350 kPa	190 mol/m^3	6.5 mK
300 K	350 kPa	140 mol/m^3	17 mK

Table 1. Best RIGT Monte Carlo quadrature sum thermodynamic temperature uncertainties

For TM11 microwave mode

CAVEATS

- Gas composition impurities, pressure head, thermomolecular pressure correction, pressure gradients along gas flow path, resonator thermal gradients, or any other systematic effects not yet included in calculations ⇒ may increase the overall T_{therm} uncertainty
- $\delta T_{\mathrm{therm}}$ calculated at a single (p, T, microwave mode) combination at a time ⇒ overall T_{therm} uncertainty may be reduced by averaging multiple measurements across modes, along isotherms, etc.
- Special efforts to push p uncertainty below NRC CMCs may reduce overall T_{therm} uncertainty

CONCLUSION

Microwave refractive index gas thermometry uncertainties within the current NRC approach, while not competitive with those of AGT [3], are likely to be small enough between 25 K – 150 K to allow useful measurements of thermodynamic temperature in this regime, to complement those made by AGT and DCGT.

REFERENCES

[1] P.M.C. Rourke & K.D. Hill, Int. J. Thermophys. **36**, 205 (2014)
[2] J. Fischer *et al.*, Int. J. Thermophys. **32**, 12 (2011)
[3] L. Pitre *et al.*, Metrologia **43**, 142 (2006)
[4] C. Gaiser *et al.*, Int. J. Thermophys. **31**, 1428 (2010)
[5] M.R. Moldover, J. Res. Natl. Inst. Stand. Technol. **103**, 167 (1998)
[6] N.J. Simon *et al.*, NIST Monograph 177 (1992)
[7] K.R.S. Shaul *et al.*, J. Chem. Phys. **137**, 184101 (2012)
[8] L.W. Bruch & F. Weinhold, J. Chem Phys. **113**, 8667 (2000)
[9] M.R. Moldover *et al.*, Metrologia **51**, R1 (2014)
[10] G. Lach *et al.*, Phys. Rev. Lett. **92**, 23301 (2004)
[11] A. Rizzo *et al.*, J. Chem. Phys. **117**, 2609 (2002)
[12] E.C. Kerr & R.H. Sherman, J. Low Temp. Phys. **3**, 451 (1970)
[13] S. Kirouac & T.K. Bose, J. Chem. Phys. **64**, 1580 (1976)
[14] M. Lallemand & D. Vidal, J. Chem. Phys. **66**, 4776 (1977)
[15] M.P. White & D. Gugan, Metrologia **29**, 37 (1992)
[16] D.F. Heller & W.M. Gelbart, Chem. Phys. Lett. **27**, 359 (1974)

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