Updates of recent work on RO physical relationships at Environment Canada

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Outline

- It was noticed years ago that physical constitutive relationships were of critical importance for the accurate interpretation of RO data
  – Equation of State of air (P,T,q) vs density
  – Refractivity vs thermodynamic variables

$$P = \rho \cdot R_d \cdot T_{virt} \cdot Z$$

$$N(P, T, x_{wv})$$

- Recommendations were issued for both
  – Air is not sufficiently ideal. Account for its compressibility.
    – Aparicio et al. 2009, JGR Atm, 114.
  – Refractivity expression is related to the above
    - Not only how accurate the expression may be
    - Most importantly, **how it is used**.
      – Aparicio and Laroche 2011, JGR Atm, 116.
- We here review those recommendations and refine them

History I: The initial symptom (2006)

- During implementation in Canada, assimilation under apparently standard assumptions shows a small but systematic negative O-B bias (all heights, -0.05%).
- Assimilation leads to negative geopotential bias (-5m)
  - Prominent against Radiosonde data.
- Not huge, but too big to be acceptable.
  - Especially since data was supposed to be unbiased.
  - Could not be used as anchor.

History II: First hints (2007)

- Not assuming that air is ideal solves (mostly) the issue.
  - Equation of state modified for nonideal effects
    - Intermolecular potentials, mostly attractive.
    - Weakly attractive between dry air molecules
    - Strongly for water-air and especially water-water
  - At given density, temperature, **pressure is slightly smaller**
    - Hydrostatic equation

$$\frac{dP}{dh} = -\rho(h) \cdot g(lat, h)$$

$$P = \rho \cdot R_d \cdot T_{virt} \cdot Z$$

- Most of O-B bias gone
- Most geopotential bias gone.

- Apparently solved BUT…
  - Shows how sensitive assimilation is
  - Opens the question**: are there other similar issues?**

History III: Refractivity (2008)

- S. Healy notes that
  - Environment Canada had chosen (Rueger, 2002) an expression that featured an unusually high k1

Elasticity of electron clouds in molecules — Induction of H_2O rotation

Dry Air — Water

$$N = 10^6 (n_{Air} - 1) = 77.6890 \frac{P_d}{T} + 71.2952 \frac{P_{wv}}{T} + 375463 \frac{P_{wv}}{T^2}$$

  - Most other centers had chosen expressions with k1=77.60
  - Yet… Rueger's work seems to have been developed carefully.

- Analysis shows that the expression
  - Does ***partially*** account for compressibility
  - Is intended for uses at low altitude
- So… all constitutive relationships had to be revisited

History IV: Revisiting refractivity

- At Env Canada, we tried to determine if enough data about refractivity existed, or new data were required.
- A microphysical model was prepared collecting all information on atmospheric constituents
  - Molar fraction
  - Molar mass
  - Molecular polarizability
  - Molecular dipole
- To obtain physical relationships to bulk properties
  - refraction index

History V: Deeper…

- Other air properties are tested for relevance
  - T, P dependent polarizability (N_2, O_2)
  - Magnetic dipole (O_2 is paramagnetic)
  - Detailed composition
    - Ar, CO_2, Ne, He, CH_4, Kr, H_2 …
    - Given a list of i substances:

Molecular polarizability Molecular dipole

$$\frac{\varepsilon_r - 1}{\varepsilon_r + 2} = \frac{1}{3\varepsilon_0}\sum_i N_i \left(\alpha_i + \frac{\mu_i^2}{3k_B T} f(\varepsilon) \right)$$

$$\frac{\mu_r - 1}{\mu_r + 2} = \frac{1}{3\varepsilon_0}\sum_i N_i \left(\alpha_{mi} + \frac{\mu_{mi}^2}{3k_B T} \right)$$

- A final air reference is produced.
  - Microphysical properties, based on **recent measurements**.
  - Atmospheric composition, based on **recent data**.
  - Functional relationship to bulk properties
- The microphysical model is applied to a wide range of air states (T, pressure, moisture)
- A "simple" fit is produced

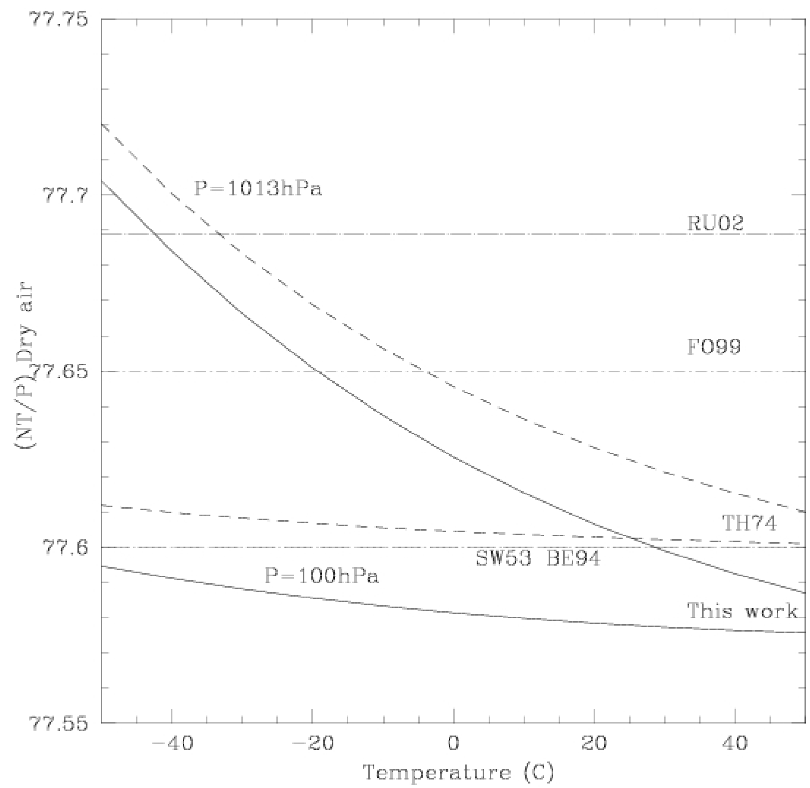
History VI: The issues

- There is no simple fit

$$N = k_1 \frac{P_d}{T} + k_2 \frac{P_{wv}}{T} + k_3 \frac{P_{wv}}{T^2}$$

$$N_{Dry} = k_1 \frac{P_d}{T}$$

- The microphysical model with pure dry air (forget water for now) **does not fit to one k1**.

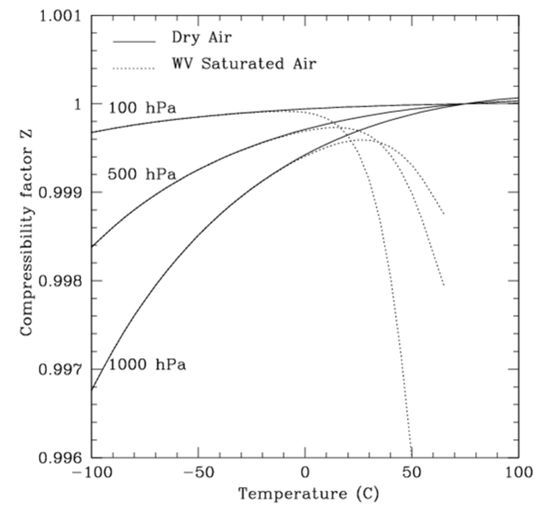


History VII: The issues (2)

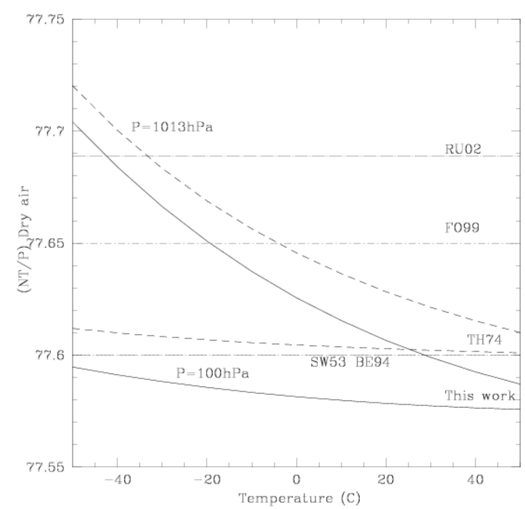
- The only comparable expression is Thayer (1974)

$$N = k_1 \frac{P_d}{T} Z_d^{-1} + \left[k_2 \frac{P_{wv}}{T} + k_3 \frac{P_{wv}}{T^2} \right] Z_{wv}^{-1}$$

- because adds compressibility to the 3-term expression
- At **surface level**, $k_1 Z_d^{-1}$ is larger, smaller above.



- The usual “k1” is **not a constant**
  – T, P (also q) dependent



History VIII: Thayer's expression

- Thayer (1974) expression $$N = k_1 \frac{P_d}{T} Z_d^{-1} + \left[k_2 \frac{P_{wv}}{T} + k_3 \frac{P_{wv}}{T^2} \right] Z_{wv}^{-1}$$
- May be acceptable for its dry term (possibly updating the coefficient)
- **Not acceptable for its moist** term
  - Why Z_{wv}^{-1} ?
  - This represents molecular adhesion **between water molecules**.
  - But water is a trace, interacts **mostly with air** Z_{dw}^{-1}
  - **"Water compressibility" was inappropriately chosen.**

- Secondly: What do P_d, P_{wv} mean?
- Are **partial pressures** proper quantities?

Partial pressures

- What do "partial pressures" mean?
  - They are **not observables**. Any conceivable thought experiment will measure other quantities, e.g.
    - Pressure of the same amount of dry air in the same container, without the vapor.
    - Pressure of the same amount of vapor in the same container, without dry air.
  - In a gas that is **not ideal** the sum of these two **is not equal** to the total pressure.
  - The likely meaning is the molar fraction in pressure units:

$$P_d = x_d P \qquad x_d + x_{wv} \equiv 1$$

$$P_{wv} = x_{wv} P \qquad P_d + P_{wv} \equiv P$$

  - But this is an assumption, we should be certain…

History IX: Begin from scratch (2010)

- Standard expressions
  - no good fit for any set of parameters
  - the exact meaning of variables is undefined

$$N = k_1 \frac{P_d}{T} + k_2 \frac{P_{wv}}{T} + k_3 \frac{P_{wv}}{T^2}$$

- A new ansatz expression was prepared
  - Using only well-defined variables
    - Acceptable: $x_d, x_{wv}, \rho_d, \rho_{wv}, T$
    - Unacceptable: P_d, P_{wv}

$$N = a_1 \rho_d + b_1 \rho_{wv} + b_2 \frac{\rho_{wv}}{T}$$

- A set a_1, b_1, b_2 is found to fit well.
- Finally, the ansatz is slightly modified:
- (allows T-dependent molecular polarizability, and O2 magnetic dipole)

$$N = a_1 \rho_d + a_2 \frac{\rho_d}{T} + b_1 \rho_{wv} + b_2 \frac{\rho_{wv}}{T}$$

History X (and final historical review)

- 2011 proposal

$$N = N_0(1 + N_0 \cdot 10^{-6} / 6)$$

$$N_0 = (222.682 + 0.069 \cdot \tau) \cdot \rho_d + (6701.605 + 6385.886 \cdot \tau) \cdot \rho_{wv}$$

$$\tau = 273.15 / T - 1$$

- Plus several details:
  - A classical 3-term ansatz on pressure **does not fit** better than existing expressions (low atm at the expense of upper, or vicev.)
  - The microphysical model allows the trace
    - For each ansatz parameter (4)
    - Identify lab measurements (~80) critical
    - Bottleneck measurements <10

Fitted ansatz parameter a

$$\partial a_i / \partial l_i$$

Lab measurement l (molecular polarizabilities, dipoles, …)

Recent work: Update & refinement

- Primary measurements & model unmodified
- Fit has been reviewed:
  - Extended atmospheric conditions
  - Variable CO2, included constraint $x_{O_2} + x_{CO_2} = const$
  - Allowance for liquid droplets, ice
- Ansatz extended:

$$N_0 = a_1\rho_d + a_2\frac{\rho_d}{T} + \boxed{a_3 x_{CO_2}\rho_d} + b_1\rho_{wv} + b_2\frac{\rho_{wv}}{T} + \boxed{b_3\rho_{wl}} + \boxed{b_4\rho_{wi}}$$

- CO2 evolves with time
- Remaining issues:
  - b3, b4 depend significantly on a form factor (flattening, orientation)
  - still working on this

Preliminary update

- 2011 proposal

$$N = N_0(1 + N_0 \cdot 10^{-6} / 6)$$
$$N_0 = (222.682 + 0.069 \cdot \tau) \cdot \rho_d + (6701.605 + 6385.886 \cdot \tau) \cdot \rho_{wv}$$
$$\tau = 273.15 / T - 1$$

- 2015 update (**preliminary**)

$$N = N_0(1 + N_0 \cdot 10^{-6} / 6)$$
$$N_0 = (222.644 + 0.108 \cdot \tau + 83.76 \cdot x_{CO_2}) \cdot \rho_d + (6702.807 + 6392.831 \cdot \tau) \cdot \rho_{wv}$$
$$+ 1415 \cdot f_{wl} \cdot \rho_{wl} + 663 \cdot f_{wi} \cdot \rho_{wi}$$
$$\tau = 273.15 / T - 1$$

  – Confirmed main ansatz
  – CO2 contribution split from dry air

$$x_{CO_2} \cdot 10^6 \cong 369 + 1.86 \cdot (y - 2000) + 0.0135 \cdot (y - 2000)^2$$

  – Still work in progress with form factors

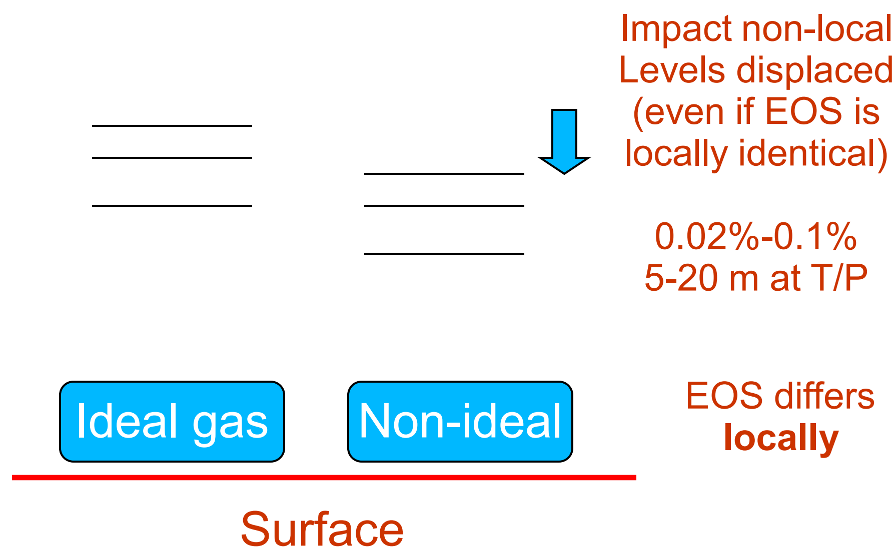
Thank you!

Appendix: Hydrostatic impact of compressibility

- Essentially, the hydrostatic equation
- We need there the equation of state (EOS)
- Already found that the deviation of EOS from ideal is non-negligible
- **Non-local**

$$\nabla P = -\vec{g}(\vec{x})\rho$$

$$P(\rho, T, x_w)$$



- 0.05% relevant for NWP if **systematic** (affects the anchor of radiances)