Inversion of the Jacobi-Porstendörfer room model for the radon progeny

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Abstract. The Jacobi-Porstendörfer (J-P) room model describes the behaviour of radon progeny in the atmosphere of a room. It distinguishes between free and attached radon progeny in air. It has been successfully used without substantial changes for nearly 40 years. There have been several attempts to invert the model approximately to determine the parameters describing the physical processes. Here, an exact solution is aimed at as an algebraic inversion of the system of six linear equations for the five unknown physical parameters k, X, R, q_b , q_a of the room model. Two strong linear dependencies in this system, unfortunately do not allow to obtain a general solution (especially not for the ventilation coefficient k), but only a parameterized one or for reduced sets of unknown parameters. More, the impossibility to eliminate one of the two linear dependencies and the departures of the measured concentrations forces to solve a set of allowed combinations of equations of the algebraic system and to accept its mean values (therefore with variances) as a result of the algebraic inversion. These results are in agreement with results of the least squares method as well as of a sophisticated modern statistical approach. The algebraic approach provides, of course, a lot of analytical relations to study the mutual dependencies between the model parameters and the measurable quantities.

Key words: Jacobi room model • inversion and invariants of the model • unattached radon daughters • attachment rate • deposition rate

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Introduction

The Jacobi room model, describing the behaviour of free and attached radon progeny in the atmosphere of a room was introduced by W. Jacobi 37 years ago [1], was worked out and broadly applied in indoor measuring by J. Porstendörfer [4, 5]. It has been successfully used up to now without substantial changes, so designating it as the J-P model is justified. There have been several attempts to invert measured data to determine the parameters describing the physical processes by approximate approaches [2, 3]. Here, an exact solution is given.

The Jacobi-Porstendörfer room model

The J-P room model for radon progeny [1, 5] is a deterministic simulation of the processes using compartments, i.e. linear processes. For steady state situation, the recurrent relations between measurable concentrations of free and attached radon progeny and the supposed parameters k, X, q_f, q_a and R are simple: Free progeny:

(1a)

(1a)
$$a_{1f} = \lambda_1 a_0 / Q_{1f}$$

(1b) $a_{2f} = \lambda_2 (a_{1f} + Ra_{1a}) / Q_{2f}$
(1c) $a_{3f} = \lambda_3 a_{2f} / Q_{3f}$

(1c)

(1d) (1e) (1f) $a_{1a} = Xa_{1f} / Q_{1a}$ $a_{2a} = (Xa_{2f} + \lambda_2 (1 - R)a_{1a}) / Q_{2a}$ $a_{3a} = (Xa_{3f} + \lambda_2 a_{2a}) / Q_{3a}$

where: a_0 – radon concentration, [Bq/m³]; a_{if} and a_{ia} – concentrations of free (index *f*) and attached (index *a*) progeny in state *i*, [Bq/m³]; *k* – ventilation rate, [h⁻¹]; *X* – attachment rate of free progeny to aerosol particles, [h⁻¹]; q_f and q_a – deposition rates of free and attached progeny to surfaces in the room, [h⁻¹]; *R* – fraction of recoiled ²¹⁴Pb atoms from aerosol particles, [1]; λ_i – transformation constants, [h⁻¹].

$$Q_{if} = \lambda_i + k + X + q_f, \quad Q_{ia} = \lambda_i + k + q_a, [h^{-1}].$$

For a set of five parameters k, X, q_f , q_a , R the six measurable concentrations of progeny a_{if} and a_{ia} can be predicted from the J-P model using relations (1).

The inversion of the Jacobi-Porstendörfer room model

Using methods of linear algebra

The task of inversion can be given more lucidly in matrix form Ax = b. Labelling the measurable progeny concentrations

$$a_{1f} = A$$
, $a_{1a} = B$, $a_{2f} = C$, $a_{2a} = D$, $a_{3f} = E$, $a_{3a} = F$

and the right sides

$$\lambda_1(a_0 - A) = a, \quad -\lambda B = b, \quad \lambda_2(A - C) = c,$$

$$\lambda_2(B - D) = d, \quad \lambda_3(C - E) = e, \quad \lambda_3(D - F) = f$$

the system of six equations for five parameters k, X, q_f , q_a , R is:

(2)
$$\begin{pmatrix} A & A & 0 & A & 0 \\ B & -A & 0 & 0 & B \\ C & C & -\lambda_2 B & C & 0 \\ D & -C & \lambda_2 B & 0 & D \\ E & E & 0 & E & 0 \\ F & -E & 0 & 0 & F \end{pmatrix} \cdot \begin{pmatrix} k \\ X \\ R \\ q_f \\ q_a \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ f \end{pmatrix}$$

For the five unknown parameters k, X, R, q_i , q_a , six linear equations are then available, between which are but two linearly dependent ones – see conditions (3a), (3b), therefore remain only four applicable equations for five unknown parameters, so system (2) cannot offer a unique solution. If input data A, B, C, D, E, F satisfy conditions (3a), (3b):

$$(3a) aE - eA \equiv 0$$

(3b)
$$(a+b)(DE-CF) + (c+d)(AF-BE) + (e+f)(AD-BC) \equiv 0$$

which are invariants of the J-P room model, the requirements of the Frobenius theorem for the system (5) are satisfied, the rank of the matrix and of the augmented matrix are after elimination of two linear equations equal but only h = 4. So, system (2) provides solution only if one of the unknowns k, q_f or q_a (not X or R^1) is chosen as a known (optional, free) parameter, i.e. a "parametric" solution is obtained.

The parameters R and X have in system (2) a privileged position among the five unknown parameters k, X, q_f , q_a , R: they are independent of the optional parameters k, q_f or q_a .

Resulting solutions of the system (2), e.g. at omission of the 5th and 6th equations are given in (4a), (4b), (4c), (4d) for various optional parameters – relations (4b) at optional q_a , relations (4c) at optional q_f , relations (4d) at optional k:

(4a)
$$X = a / A + [(a+b)D - (c+d)B] / \Delta,$$
$$R = (aC - cA) / (\lambda, AB)$$

(4b)
$$k = [(a+b)C - (c+d)A] / \Delta - q_a,$$

 $q_f = [-(a+b)(C+D) + (c+d)(C+D)] / \Delta + q_a$

(4c)
$$k = [-(a+b)D + (c+d)B] / \Delta - q_f,$$

 $q_a = [(a+b)(C+D) - (c+d)(A+B)] / \Delta - q_f$

(4d)
$$q_f = [-(a+b)D + (c+d)B]/\Delta - k,$$

 $q_a = [(a+b)C - (c+d)A]/-k$

where: $\Delta = BC - AD$.

Satisfying conditions (3a), (3b), however happen evidently only at that time, if as input values A, B, C, D, E, F calculated data are used obtained from relations (1) for arbitrarily chosen sets of the five parameters k, X, q_f , q_a , R, which is, as a matter of fact, only checking of the algorithm. Unfortunately however for experimentally gained results A, B, C, D, E, F, the conditions (3a), (3b) for the existence of a unique "parametric" solution are never satisfied, so that the rank of the matrix and of the augmented matrix are not equal and the aforesaid $\binom{6}{4} = 15$ combinations of equations are possible, between which six are forbidden: one containing both the 3rd and 4th equation (it would eliminate the parameter R) and five containing simultaneously the 1st and 5th equation (which are evidently linearly dependent and reduce the rank to h = 3). This leads to nine (mostly) different results for the set of four unknown parameters (and 1 free one). The range of those distinctnesses will be shown in Table 2, using experimental data of Table 1 obtained in a radon chamber of National Radiation Protection Institute (NRPI), Praha.

Providing that especially (or alone?) the value E "spoil" the inversion, it is possible to determine substitute value, according to condition (3a). Results of inversion are given in Table 2 for the full number of combinations of equations for both sets of measurements.

It would be difficult to give rational priorities which combination of equations have to be used (e.g. the first four equations containing measurements with higher accuracy) and which not (e.g. the last two equations containing measurements with less accuracy) as arguments can be given, on the contrary, also (important,

| | | | | , , |) -)) | , | | | | | |
|-----|-------|------|-------|-------|---------|-------|--------|-------|----------|----------|-------------------|
| Set | a_0 | k | A | В | С | D | Ε | F | Eq. (3a) | Eq. (3b) | $E/E_{\rm theor}$ |
| 1 | 884 | 0.35 | 0.498 | 0.335 | 0.100 | 0.423 | 0.0510 | 0.395 | 6.8 | 0.80 | 3.9 |
| 2 | 928 | 0.35 | 0.503 | 0.318 | 0.066 | 0.484 | 0.0354 | 0.402 | 7.0 | 0.95 | 3.9 |

Table 1. Results of five sets of measurements A, B, C, D, E, F standardized on unit radon concentration

Table 2. Variability of the nine solutions of algebraic inversion in the case of known ventilation rate k; E_{theor} is used (i.e. aE = eA)

| | | Set no. 1 | | |
|----------|------|-----------|---------|-------|
| Used eq. | X | R | q_{f} | q_a |
| 2346 | 9.5 | 1.17 | 2.5 | 0.12 |
| 1346 | 11.2 | 1.45 | 2.3 | 0.18 |
| 1246 | 9.5 | 1.17 | 3.9 | 0.12 |
| 1236 | 9.5 | 1.45 | 3.9 | 0.12 |
| 1234 | 9.2 | 1.45 | 4.2 | -0.28 |
| 3456 | 11.2 | 1.45 | 2.3 | 0.18 |
| 2456 | 9.5 | 1.17 | 3.9 | 0.12 |
| 2356 | 9.5 | 1.45 | 3.9 | 0.12 |
| 2345 | 9.2 | 1.45 | 4.2 | -0.28 |
| Mean | 9.8 | 1.36 | 3.45 | 0.042 |
| Variance | 8% | 10% | 25% | 440% |
| | | Set no. 2 | | |
| Used eq. | X | R | q_{f} | q_a |
| 2346 | 9.0 | 0,06 | 1.4 | 0.28 |
| 1346 | 12.2 | 0.42 | 0.9 | 0.35 |
| 1246 | 9.0 | 0.06 | 4.1 | 0.28 |
| 1236 | 9.0 | 0.42 | 4.1 | 0.28 |
| 1234 | 8.8 | 0.42 | 4.4 | -0.12 |
| 3456 | 12.2 | 0.42 | 0.9 | 0.35 |
| 2456 | 9.0 | 0.06 | 4.1 | 0.28 |
| 2356 | 9.0 | 0.42 | 4.1 | 0.28 |
| 2345 | 8.8 | 0.42 | 4.4 | -0.12 |
| Mean | 9.67 | 0.30 | 3.15 | 0.21 |
| Variance | 15% | 60% | 50% | 90% |

e.g., are the consequences of the J-P model on the RaC, i.e. the last two Eqs. (1c), (1f)). Table 2 shows that the average value and its variance can be a good approach to get an estimate of the involved parameters.

Similar conclusions can be obtained in cases when activities of radon progeny on surfaces are measured as well as thoron progeny in air and on surfaces.

Using statistical methods

Superfluous equations (but two of them are linearly dependent) in the task given above offer the application

of statistical methods but only for given sets of measured results. A multiple linear regression analysis without constraints gives acceptable results. Linear programming can be used also.

The most common approach for these tasks is the least-squares multiple regression method. Applied to the general case of system (2) with six equations and five unknowns only parametric solutions can be obtained plus an estimation of uncertainty (Table 3).

Compared with results of algebraic inversion in Table 2 satisfactory agreement can be stated regardless of the minimal degree of freedom f = 1 and the existence of two linear dependencies. The regression

Table 3. Results of the least-squares method in the case of unknown ventilation coefficient k for two sets of measured data

| Set no. | $X \pm s_X$ | | $R \pm s_R$ | (k | $\pm s_k$) + ($q_a \pm s_{qa}$ | .) | $(q_f =$ | $\pm s_{qf}$) – ($q_a \pm$ | (s_{qa}) |
|-------------|----------------|-----------|-----------------|--|----------------------------------|------------|--------------------------------------|------------------------------|----------------|
| 1 | 9.43 ± 0.1 | 15 | 1.35 ± 0.9 | (0.35 | $\pm 0.13) + (q_a \pm$ | S_{qa}) | (3.96 = | $\pm 0.29) - (q_a)$ | $\pm s_{qa}$) |
| 2 | 8.93 ± 0.1 | 1/ | 0.31 ± 0.12 | $0.12 \qquad (0.48 \pm 0.14) + (q_a \pm s_{qa})$ | | | $(4.04 \pm 0.31) - (q_a \pm s_{qa})$ | | |
| Table 3a. T | he correlatio | on matrix | of parameters | | | | | | |
| Set no. 1 | X | R | $k + q_a$ | $q_f - q_a$ | Set no. 2 | X | R | $k + q_a$ | $q_f - q_a$ |
| X | - | -0.21 | 0.64 | -0.82 | X | _ | -0.24 | 0.58 | -0.81 |
| R | -0.21 | - | -0.47 | 0.39 | R | -0.24 | - | -0.52 | 0.41 |
| $k + q_a$ | 0.64 | -0.64 | - | -0.82 | $k + q_a$ | 0.58 | -0.52 | - | -0.78 |
| $q_f - q_a$ | -0.83 | 0.39 | -0.82 | _ | $q_f - q_a$ | -0.81 | 0.41 | -0.78 | _ |

provides also a reasonable correlation matrix showing strong relations between the parameters mutually.

Or, one can use a bit more sophisticated regression approach in which observations $y = (a_0, A, B, C, D, E, F, k)$ are only implicit functions of the parameters of interest (standard errors of the observations are then also functions of the unknown parameters and can be approximately obtained via delta method, or local linearization). Linear dependency among parameters has to be solved then (e.g. via reparametrization and estimation of certain linear combination of parameters not all parameters of interest).

Alternatively, one can use Bayesian (hierarchical) modelling to get posterior estimates of the five parameters of interest, $\underline{\theta} = (k, X, q_f, q_a, R)$ ' from the measured data and flat (or non-informative) prior on $\underline{\theta}$. Measured data $\underline{y} = (a_0, A, B, C, D, E, F, k)$ are essentially assumed to be normally and independently, but heteroscedastically distributed, given the parameters. In fact, we assume:

$$\begin{aligned} a_0 &| \underline{\theta} \sim N(m_{a0}, s_{a0}^2), A | \underline{\theta} \sim N(m_A, s_A^2), \\ B &| \underline{\theta} \sim N(m_B, s_B^2), C | \underline{\theta} \sim N(m_C, s_C^2), \\ D &| \underline{\theta} \sim N(m_D, s_D^2), E | \underline{\theta} \sim N(m_E, s_E^2), \\ F &| \underline{\theta} \sim N(m_F, s_F^2), k | \underline{\theta} \sim N(k, s_k^2) \end{aligned}$$

independently, where:

- $s_{a0}^2, ..., s_F^2, s_k^2$ are given by the measurement uncertainties (their standard errors). These are known and come with the measured values (they are computed by metrological methods by a specialist conducting y measurements),
- means (in fact, we mean) of the normal observation distributions are given as

$$\begin{split} m_{A} &= \lambda_{1} m_{a_{0}} / Q_{1f} \\ m_{B} &= X m_{B} / Q_{1a} \\ m_{C} &= (\lambda_{2} m_{A} + R \lambda_{2} m_{B}) / Q_{2f} \\ m_{D} &= (X m_{C} + (1 - R) \lambda_{2} m_{B} / Q_{2a} \\ m_{E} &= \lambda_{3} m_{D} / Q_{3f} \\ m_{F} &= (X m_{E} + \lambda_{3} m_{D}) / Q_{3a} \end{split}$$

these are functions of the parameters $\underline{\theta}$ (so that their posterior distributions can be obtained, if needed),

- for m_{a_0} , very flat normal prior was assumed,
- priors for the parameters were independent, as follows:
- $k \sim Unif(0,1), X \sim Unif(0,100), q_f \sim Unif(0,100), q_a \sim Unif(0,100), R \sim Unif(0,1).$

Model is fitted by Markov chain Monte Carlo (MCMC) method simulations (to get a sample of $\underline{\theta}$ posterior, we use MCMC Gibbs sampling with 100 000 burn-in period). Sample of 100 000 is then used with 1:10 thinning – i.e. effectively 10 000 values with reasonably small autocorrelation. Point estimates are obtained as posterior means and estimates of their uncertainties as posterior standard deviations. The following Table 4 gives the results for five sets of measurements conducted in an experimental room of the NRPI under similar conditions (constituting basically random replications).

Good agreement with physically plausible ranges is reached for parameters X and q_f , not so good for q_a but discrepancies are for R between statistical and algebraic approaches.

Usefulness of the inversion of the J-P room model

It can be shown that the deterministic J-P model is exactly invertible only if beside of free and attached radon progeny concentrations in the room air also the contamination with radon progeny of room surfaces is measured. But the latter is a laborious task and only few studies in laboratory conditions have been realized [3]. Therefore, in practice only the air concentrations are available in common and the incomplete inversion or the shown regression approach has to be used. It is shown that also with a known ventilation rate (measured by an independent method) exact inversion cannot be reached.

The analytical solutions (4) show nice symmetry, but this is of low value for practice, e.g. the results for k and q_f will be rightfully dependent on the estimation of q_a . At least the relations enable:

- Mainly from sets of measured results A, B, C, D, E, F in field studies to estimate a set of the five parameters k, X, R, q_f, q_a which are directly related to the environment of the room.
- To evaluate the preciseness of sets of measured data using the conditions (3).
- To study in a more general way the power of dependence between A, B, C, D, E, F and k, X, R, q_f, q_a.
- To compare previously published approximate solutions.

Discussion and conclusions

The presumptions of the J-P model are homogeneous distribution of radon and its progeny in the volume of the room as well as homogeneous contamination of the

| Table 4. Posterior means (a) | and standard | deviations in | %)/results | of inversion | with know | 'n k |
|------------------------------|--------------|---------------|------------|--------------|-----------|------|
|------------------------------|--------------|---------------|------------|--------------|-----------|------|

| Demonstration | Set no. | | | | | | | | |
|---------------|-----------------|-----------------|----------------|-----------------|----------------|--|--|--|--|
| Parameter | 1 | 2 | 3 | 4 | 5 | | | | |
| k | 0.35 (5) | 0.35 (5) | 0.35 (5) | 0.35 (5) | 0.20 (5) | | | | |
| Χ | 8.29 (9)/9.2 | 8.49 (10)/8.9 | 11.2 (6)/13 | 15.8 (11)/17 | 20.3 (5)/22 | | | | |
| q_f | 2.67 (35)/4.2 | 2.16 (38)/4.4 | 2.72 (36)/2.5 | 3.38 (46)/5.6 | 4.05 (30)/3.5 | | | | |
| \tilde{q}_a | 0.19 (58)/0.06 | 0.27 (15)/0.02 | 0.27 (39)/0.07 | 0.15 (60)/0.09 | 0.20 (34)/0.13 | | | | |
| Ŕ | 0.80 (19)/-0.28 | 0.20 (79)/-0.12 | 0.91 (9)/0.33 | 0.71 (29)/-0.35 | 0.93 (7)/0.23 | | | | |
| DIC* | 64.3 | 63.6 | 59.9 | 61.8 | 58.6 | | | | |

*DIC – deviance information criterion (the smaller the better).

surfaces of the room and also steady state conditions. This is mostly not fulfilled in field studies, better is in radon chambers for calibration using air mixing. The condition of homogeneity is broken especially by the short-lived ²¹⁸Po and may be a correction factor can be introduced to fulfil the invariants (3a), (3b).

The theoretically founded estimates for the parameters X, R, q_j , q_a are also only approximations for the situation in the measured spot and cannot reflect the complicated conditions in the whole room in actual and occupied rooms. Therefore, values of k, X, R, q_f , q_a obtained from measured quantities in field studies by inversion give averaged actual estimates. These estimates can be used to explain the differences in actual situations (smokers x non-smokers, city x countryside etc.) in terms of aerosol concentrations or depositionpotentials. Unfortunately, the certainty of these estimates is limited by the optional parameter and by the uncertainties of the measured quantities.

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