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Diffusion of Impurities in the MDT Gas System

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Abstract

The gas in the MDT chambers will contain impurities from outgassing, inward leaks, action of radiation and other sources. An understanding of how these impurities spread through diffusion can help with certain design choices: gas flow rate, connecting tube diameter, how many tubes to connect in series and maybe others. This note gives the basic equation that governs diffusion in a flowing gas, and solves some representive cases to give a feel for how important the effects are in specific circumstances.

1 Steady state differential equation for diffusion in a flowing gas

Consider an impurity in the MDT gas. We treat the problem in 1 dimension, ignoring effects across the tube. We want to know the density of the impurity, $n(x)$, along the tube.

The current j_d due to diffusion is related to the impurity density from Fick's law by

$$j_d = -D\frac{\partial n}{\partial x}$$

where D is the diffusion coefficient.

The current j_v due to the MDT gas flow velocity v (taken to be in the positive x direction) is

$$j_v = vn$$

The total current is the sum of these two:

$$j = -D\frac{\partial n}{\partial x} + nv \tag{1}$$

Consider a cylinder of length $\mathrm{d}x$ and cross-sectional area S, with incoming current j and outgoing current $j + \mathrm{d}j$. The accumulation of impurity in the cylinder is

$$-\mathrm{d}jS = -\frac{\partial j}{\partial x}S\mathrm{d}x.$$

But this accumulation rate plus any net rate of production of impurity $Q(x)$ is the same as the rate of change of impurity in the volume element, i.e.

$$\frac{\partial n}{\partial t}S\mathrm{d}x = -\frac{\partial j}{\partial x}S\mathrm{d}x + QS\mathrm{d}x$$

Substituting for j from (1) and cancelling the common volume element $S\mathrm{d}x$ gives

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} - v\frac{\partial n}{\partial x} + Q$$

This is the equation of motion for the impurity. It is time dependent; we look for the steady state solution $\partial n/\partial t = 0$, giving

$$\frac{\partial}{\partial x}(D\frac{\partial n}{\partial x} - vn) + Q = 0$$

Integrating from some convenient point $x = a$ gives

$$D\frac{\partial n}{\partial x} - vn + \int_a^x Q(x')\mathrm{d}x' = \text{const}$$

Conservation of impurity implies

$$j(x) - j(a) = \int_a^x Q(x')\mathrm{d}x',$$

i.e. what goes in at a plus production upto x comes out at x. Comparison with equation (1) then shows the constant is $-j(a)$.

Hence, at the steady state, we have to solve the equation

$$D\frac{\partial n(x)}{\partial x} - vn(x) + \int_a^x Q(x')\mathrm{d}x' = -j(a) \tag{2}$$

2 Application Examples

2.1 Case 1: Leak at inlet end

Consider a tube starting at $x = 0$ and ending at $x = L$, with clean gas coming in at x = 0. Suppose the endplug at the inlet has a leak rate q with no other sources of impurity. Then $Q(x)\mathrm{d}x = q$ for $x = 0$ and 0 elsewhere,

$$\int_0^x Q(x')\mathrm{d}x' = q \text{ for } x \geq 0$$

Furthermore, suppose the inlet tube is so narrow that no impurity can back-diffuse up it, i.e. $j(0) = 0$. Then equation (2) becomes

$$D\frac{\partial n(x)}{\partial x} - vn(x) + q = 0$$

with solution

$$n(x) = Ae^{\frac{v}{D}x} + \frac{q}{v}$$

We use the boundary condition that all q comes out the far end, so that $j(L) = vn(L) = q$ or

$$vAe^{vL/D} + q = q$$

so $A = 0$ and the solution is

$$n(x) = \frac{q}{v}$$

One sees the tube fills up with an equal concentration of impurity along its length, independantly of the diffusion coefficient. Higher leak rates give higher impurity levels; higher flows give lower impurity levels.

The steady-state level is proportional to the leak rate and inversely proportional to the flow rate.

2.2 Case 2: Leak at outlet end

Suppose we have no leak at the inlet, but a leak at the outlet end, all other things remaining the same. Now

$$\int_0^x Q(x')\mathrm{d}x' = 0 \text{ for } 0 \leq x < L$$

and

$$\int_0^x Q(x')\mathrm{d}x' = q \text{ for } x = L$$

So (2) reduces to

$$D\frac{\partial n}{\partial x} = vn(x)$$

with solution

$$n(x) = Ae^{\frac{v}{D}x}$$

The boundary condition is $vn(L) = q$ hence

$$A = \frac{q}{v}e^{-\frac{v}{D}L}$$

So the solution is

$$n(x) = \frac{q}{v}e^{\frac{v}{D}(x-L)}$$

One sees that for very high diffusion, this reduces to the same solution as case 1: the tube fills up with a constant level of impurity. At low diffusion, the level of impurity is a maximum at L and falls exponentially towards the inlet end of the tube, to a level

$$\frac{q}{v}e^{-\frac{v}{D}L}$$

Now one sees what is meant by "low" or "high" diffusion in the case of drift tubes: Low diffusion is when vL/D is large, so that the concentration is very low at the inlet end; high diffusion is when D is large compared to vL, so that the concentration at the inlet end is almost the same as at the leaking outlet end. For example, we have $L = 4$ m tubes with one volume exchange a day giving $vL = 1.9$ cm^2/s. This can be compared to the diffusion coefficient for water in air of 0.238 cm^2/s at 1 atmosphere pressure and 8^o C. $D \propto T/P$ so for our tubes $D = 293/281 \times 1/3 \times 0.238 = 0.083$ cm^2/s. In other words, at the planned ATLAS flow rate, our diffusion is a negligibly small effect inside tubes. The impurity concentration at the inlet end will be down a factor $e^{1.9/0.083} \approx 10^{10}$ on that at the leaking outlet end. (Note: at such high reductions other effects would dominate, such as impurity creeping along the walls where the gas velocity is very low – this would require modelling the problem in 2D, which could be done in cylindrical coordinates with Bessel functions for the radial part of the solution). This factor is extremely sensitive to flow rate: if we reduced our exchange rate to once per ten days (proposed as an alternative to purification of the gas) diffusion starts to become significant: this factor reduces to 10.

2.3 Case 3: Production of impurities along the wire

Some impurities (e.g. ethene in DATCHA gas) are produced along the wire by irradiation. Suppose that instead of leaks we have a constant rate of production of impurity per unit length of wire $\hat{q}$ so that

$$\int_0^x Q(x')\mathrm{d}x' = \hat{q}x$$

and equation (2) becomes

$$D\frac{\partial n(x)}{\partial x} - vn(x) + \hat{q}x = 0 \tag{3}$$

with solution

$$n(x) = \frac{\hat{q}}{v}x + \frac{D\hat{q}}{v^2} + Ae^{\frac{v}{D}x}$$

The boundary condition is $vn(L) = \hat{q}L$ (all that goes in comes out) giving

$$A = -\frac{D\hat{q}}{v^2}e^{-\frac{v}{D}L}$$

and so the solution is

$$n(x) = \frac{\hat{q}}{v}x + \frac{D\hat{q}}{v^2}(1 - e^{\frac{v}{D}(x-L)})$$

For high diffusion ($vL/D \ll 1$) we can expand the exponent to first order and the solution reduces to

$$n(x) = \hat{q}L/v$$

i.e. the tube fills with a constant level of impurity.

For low diffusion, $n(x) = \hat{q}x/v$ (e.g. by setting D to zero in equation (3)), i.e. the impurity builds up linearly along the tube. At intermediate rates of diffusion, the level starts off non-zero at $x = 0$ and rises to $\hat{q}L/v$ at the exit end.

It is interesting to consider what happens when several tubes are connected in series, which has been suggested to make mechanical assembly easier. The effective tube length L increases, but, if we maintain one volume exchange per day, so does the gas velocity; the result is that the impurity at the exit of the last tube remains the same, independantly of the number of tubes in series, and independantly of the diffusion coefficient. This is interesting for aging considerations.

If the impurities affect r(t) and diffusion is such that the first tube in the chain has a much lower concentration of impurities than the last, then putting tubes in series would be a very bad way of assembling chambers: tubes in the same autocalibration zone would have different r(t) relationships, making autocalibration practically impossible. Leaks and outgassing (especially of water) would also be bad for autocalibration. Most regimes of diffusion would give problems, e.g. (i) with low diffusion ($vL/D \gg 1$) the concentration of impurities increases approximately linearly along the whole chain; (ii) with high diffusion in the drift tubes ($vL/D \ll 1$) but low diffusion in the narrow connecting tubes, the concentration increases in steps at each connector-tube in the chain.

2.4 Case 4: Inter-connecting tubes

We see from case 2 that a tube with a concentration n(L) at its exit due to a leak there has n(x) decreasing exponentially towards the inlet, with decay constant v/D per unit length. In the connecting tubes, v is much higher (by

the ratio of the tube areas), but the length is much lower, say 40 mm instead of 4 m. So a connecting tube of 3 mm diameter and 40 mm long would have the same reduction in n as a 4 m long, 30 mm diameter tube. This is a considerable reduction, and suggests that for "normal" leaks, outgassing, and radiation production of impurities, back-diffusion is not a problem and there is no need to put special effort into making the connecting tubes especially small; probably they will be about 1 mm inner diameter for convenience and this should be small enough from the point of view of back diffusion and large enough to not give a significant pressure drop. Still, there may be other reasons to go smaller, e.g. to ensure equal flows in all tubes in an MDT.

We now see the justification for the assumption in cases 1 to 3 that nothing diffuses out the inlet end ($j(0) = 0$). Nonetheless, we can calculate the back diffusion easily enough by not making this assumption. Imagine one tube in an MDT has a large leak and therefore a high concentration of impurities. Suppose the impurity concentration in the gas distributor remains at 0 because whatever back-diffuses into the distributor is rapidly swept away through the other tubes. We consider the gas connector between the tube and distributor to start at 0 and end at L; $n(0) = 0$. $Q(x) = 0$ and equation 2 reduces to

$$D\frac{\partial n(x)}{\partial x} - vn(x) = -j(0)$$

with solution

$$n(x) = Ae^{(\frac{v}{D}x)} + j(0)/v$$

The boundary condition $n(0) = 0$ gives $A = -j(0)/v$. Considering the point $x = L$ gives

$$\frac{j(0)}{v} = -\frac{n(L)}{e^{\frac{v}{D}L} - 1}$$

Hence

$$n(x) = n(L)\frac{e^{\frac{v}{D}x} - 1}{e^{\frac{v}{D}L} - 1}$$

To put some numbers in, consider 1 mm diammeter connecting tubes 40 mm long, with 1 % O_2 at the drift tube end: this is $n(L) = 6 \times 10^{15}$ molecules per cm of connector-tube at 3 bar. The velocity at 1 exchange per day of a 4 m tube is $400/(24 \times 60 \times 60) \times 30^2 = 4$ cm/s. The diffusion coefficient of oxygen in air is about 0.2 cm^2/s, so we take $D = 0.2/3$ cm^2/s for argon at 3

bar. This gives

$$j(0) = -vn(L)/(e^{\frac{v}{D}L} - 1) \approx -10^{-88}\text{molecules per s}$$

i.e. back diffusion is totally negligible (the minus sign indicates the net flow is up-stream).

Take care though; note the extremely strong dependence (exponential) of this rate on the connecting tube diameter: if we used 6 mm tube, the gas velocity is 36 times slower and the flow rate of oxygen becomes greater than 10^{15} molecules per second: a change of over 100 orders of magnitude for a factor 6 change in the tube diameter.

3 Summary

The basic equation for diffusion has been solved for various cases, under certain specific conditions.

The effect of an inward leak at the outlet end was considered in Case 2, and it was shown that the impurity hardly spreads upstream along the tube at all.

Production of impurity along the wire was discussed in Case 3. It was shown (Case 2) that diffusion is small, so that for MDTs the concentration builds up steadily along the tube. Hence putting several tubes in series will mean tubes in the same autocalibration zone will have very different levels of impurities. If the impurity affects the r(t) relationship this would raise problems for autocalibration. If the diffusion had been high, then the concentration of impurity would have tended to equalise within a tube but increase at each tube boundary along the chain of tubes.

For aging, the concentration of impurity at the exit of the last tube is independant of the number of tubes in series. One can speculate about what effect this has: with all tubes in parallel, they all have a high concentration at their end and are therefore equally likely to die. With tubes in series, only the last tubes in the chain would see the highest concentration of impurity, and so only they would die (but would be more thoroughly dead!).

Back diffusion along the interconnecting tubes was considered in Case 4. With 1 mm inner diameter connectors 4 cm long, back diffusion into the inlet distributor is totally negligible. But this parameter must be kept small, say less than 2 mm, or back-diffusion could become a problem.

It would be interesting to check this model with an oxygen meter at various flow rates of argon along a tube with different leaks. Note that other effects such as creeping of molecules along the tube walls can become much more important than back-diffusion in the bulk of the gas.