Calculations for abiotic methane oxidation

Lennon et al.

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Set working directory

```
rm(list=ls())
getwd()
```

```
## [1] "/Users/lennonj/GitHub/radiolyticCH4/code/theory"
```

```
#setwd("~/GitHub/radiolytic")
```

Energy generated from radon decay

First step in the radon decay chain is the α-decay of a single ^{222}Rn atom to ^{218}Po. From Ruzer (2004), Table 14.1, page 365 in "Aerosols Handbook: Measurement, Dosimetry, and Health Effects" editors L.S. Ruzer and N.H. Harley. CRC Press.

```
# Megaelectron-volts (MeV) from Rn decay
Rn.decay <- 5.486

# Conversion factro from MeV to kilojoules (kJ)
MeV.kJ <- 1.602 * 10^-16

# kJ of energy in 222Rn to 218Po decay
print (MeV.kJ * Rn.decay)
```

```
## [1] 8.789e-16
```

Energy required to generate a methyl radical from CH_4

```
# Bond energy (kJ/mol) to break C-H in CH4 (Smith and March 2007)
bond <- 416

# Avogadro's number
A <- 6.023 * 10^23

# Energy needed to generate a methyl radical
 print(methyl.rad <- bond/A)
```

```
## [1] 6.907e-22
```

How many CH_4 molecules are there in 2 ppm CH_4 of air?

```
# assumed ppm of CH4 in air
CH4.air.ppm <- 2

# assumed conctrnation of CH4 in air
CH4.air.conc <- CH4.air.ppm/10^6

# Number of molecules in 1 mole of air
mol.air <- 6.023 * 10^23

# Number of molecules of CH4 in 1 mole of air at 2 ppm CH4
CH4.molec.mol.air <- mol.air * CH4.air.conc

# Number of liters in a mole
L.mole <- 22.4

# Liters in a cubic meter (m^3)
L.cm3 <- 1000

# Molecules of CH4 in 1 m^3 of air at 2 ppm CH4
CH4.molec.m3.air <- (CH4.molec.mol.air / L.mole) * L.cm3

print(CH4.molec.m3.air)
```

```
## [1] 5.378e+19
```

How many CH_4 molecules can be oxidized via direct contact with α particles?

```
# Reported 222Rn concentration (Bq m^-3) in Castanar Cave; decays per second
Rn <- 35000

# Time to oxidize all CH4 molecules in 2 ppm CH4
CH4.time.secs <- CH4.molec.m3.air/Rn

CH4.time.mins <- CH4.time.secs/60

CH4.time.hrs <- CH4.time.mins/60

CH4.time.days <- CH4.time.hrs/24

CH4.time.yrs <- CH4.time.days/365

print(format(CH4.time.yrs, scientific = TRUE))
```

```
## [1] "4.872e+07"
```

How many CH_4 molecules can be oxidized via ions and radicals generated via α particles and water vapor?

```
# Ions generated assuming 1 alpha decay generates 10^7 total ions
# From Fernandez-Cortes et al. (2015) page 8, column 2
ions <- 4.31 * 10^5

# Time to oxidize all CH4 molecules in 2 ppm CH4
CH4.time.ions.sec <- CH4.molec.m3.air/(Rn*ions)

CH4.time.ions.min <- CH4.time.ions.sec/60

CH4.time.ions.hrs <- CH4.time.ions.min/60

CH4.time.ions.day <- CH4.time.ions.hrs/24

CH4.time.ions.yrs <- CH4.time.ions.day/365

print(format(CH4.time.ions.yrs, scientific = FALSE))
```

```
## [1] "113"
```