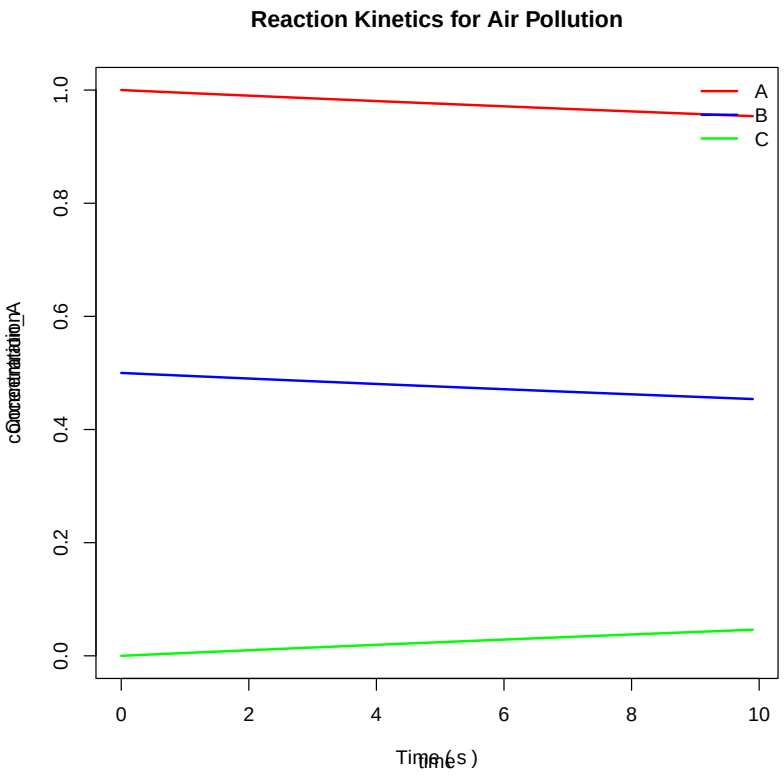
# *Reaction Kinetics for Air Pollution*

*December 15, 2023*

Here's an example R code for simulating reaction kinetics in the context of air pollution using a simple chemical reaction model. In this example, I'll use the well-known reaction of pollutants A and B reacting to form a product C. This is a simplified model, and the actual chemical reactions in the atmosphere can be more complex.

```r
# Reaction Kinetics for Air Pollution

# Parameters
rate_constant <- 0.01   # Reaction rate constant
initial_concentration_A <- 1.0  # Initial concentration of pollutant A
initial_concentration_B <- 0.5  # Initial concentration of pollutant B
initial_concentration_C <- 0.0  # Initial concentration of product C

# Simulation parameters
dt <- 0.1    # Time step
num_steps <- 100   # Number of time steps

# Initialize concentrations
concentration_A <- rep(0, num_steps)
concentration_B <- rep(0, num_steps)
concentration_C <- rep(0, num_steps)

concentration_A[1] <- initial_concentration_A
concentration_B[1] <- initial_concentration_B
concentration_C[1] <- initial_concentration_C

# Reaction kinetics simulation loop
for (step in 2:num_steps) {
  # Reaction kinetics
  dA_dt <- -rate_constant * concentration_A[step - 1] * concentration_B[step - 1] * dt
  dB_dt <- -rate_constant * concentration_A[step - 1] * concentration_B[step - 1] * dt
  dC_dt <- rate_constant * concentration_A[step - 1] * concentration_B[step - 1] * dt

  # Update concentrations
  concentration_A[step] <- concentration_A[step - 1] + dA_dt
  concentration_B[step] <- concentration_B[step - 1] + dB_dt
  concentration_C[step] <- concentration_C[step - 1] + dC_dt
}

# Plotting the results
```

```
time <- seq(0, (num_steps - 1) * dt, by = dt)

plot(time, concentration_A, type = 'l', col = 'red', lwd = 2, ylim = c(0, max(initial_concentration_A, ini
lines(time, concentration_B, type = 'l', col = 'blue', lwd = 2)
lines(time, concentration_C, type = 'l', col = 'green', lwd = 2)

legend('topright', legend = c('A', 'B', 'C'), col = c('red', 'blue', 'green'), lwd = 2, bty = 'n')
title(main = 'Reaction Kinetics for Air Pollution')
xlabel <- expression('Time (' ~ s ~ ')')
ylabel <- expression('Concentration')
title(xlab = xlabel, ylab = ylabel)
```




*with temperature*

```
# Reaction Kinetics for Air Pollution with Temperature

# Parameters
initial_concentration_A <- 1.0  # Initial concentration of pollutant A
initial_concentration_B <- 0.5  # Initial concentration of pollutant B
```

```
initial_concentration_C <- 0.0  # Initial concentration of product C

# Simulation parameters
dt <- 0.1    # Time step
num_steps <- 100   # Number of time steps

# Temperature parameters
initial_temperature <- 300  # Initial temperature in Kelvin
temperature_increase_rate <- 1  # Rate of temperature increase over time
activation_energy <- 20  # Activation energy for the reaction

# Function to calculate the rate constant based on temperature
calculate_rate_constant <- function(temperature) {
  return(exp(-activation_energy / (8.314 * temperature)))
}

# Initialize concentrations and temperature
concentration_A <- rep(0, num_steps)
concentration_B <- rep(0, num_steps)
concentration_C <- rep(0, num_steps)
temperature <- rep(0, num_steps)

concentration_A[1] <- initial_concentration_A
concentration_B[1] <- initial_concentration_B
concentration_C[1] <- initial_concentration_C
temperature[1] <- initial_temperature

# Reaction kinetics simulation loop
for (step in 2:num_steps) {
  # Temperature increase over time
  temperature[step] <- initial_temperature + temperature_increase_rate * (step - 1) * dt

  # Reaction kinetics with temperature dependence
  rate_constant <- calculate_rate_constant(temperature[step])

  dA_dt <- -rate_constant * concentration_A[step - 1] * concentration_B[step - 1] * dt
  dB_dt <- -rate_constant * concentration_A[step - 1] * concentration_B[step - 1] * dt
  dC_dt <- rate_constant * concentration_A[step - 1] * concentration_B[step - 1] * dt

  # Update concentrations
  concentration_A[step] <- concentration_A[step - 1] + dA_dt
  concentration_B[step] <- concentration_B[step - 1] + dB_dt
  concentration_C[step] <- concentration_C[step - 1] + dC_dt
```

```
}

# Plotting the results
time <- seq(0, (num_steps - 1) * dt, by = dt)

par(mfrow = c(2, 1), mar = c(4, 4, 2, 2), oma = c(0, 0, 2, 0))
plot(time, concentration_A, type = 'l', col = 'red', lwd = 2, ylim = c(0, max(initial_concentration_A, ini
lines(time, concentration_B, type = 'l', col = 'blue', lwd = 2)
lines(time, concentration_C, type = 'l', col = 'green', lwd = 2)
legend('topright', legend = c('A', 'B', 'C'), col = c('red', 'blue', 'green'), lwd = 2, bty = 'n')
title(main = 'Reaction Kinetics for Air Pollution')

plot(time, temperature, type = 'l', col = 'orange', lwd = 2, ylim = c(initial_temperature, max(temperature
title(main = 'Temperature Profile')
xlabel <- expression('Time (' ~ s ~ ')')
ylabel <- expression('Temperature (K)')
title(xlab = xlabel, ylab = ylabel)
```