

## 7 - Exploring Features of a Dynamic Equilibrium

We extend the dice simulation found at <https://www.jon.hk/app/kineqmsim/> to explore some features of a dynamic equilibrium. Choose the *competition* tab. You will need to reset the simulation in every part (unless otherwise instructed).

### 1. Microscopic vs Macroscopic

(a) Run a simulation with the following conditions: dieCount = 3000, initialRemain = 3000, dieSide = 100, forwardConditions = 3, backwardConditions = 1, mystery = 500.

i. What is the average red:gray ratio between 140–160 rounds?

i. \_\_\_\_\_

ii. What is the average red:gray ratio between 200–220 rounds?

ii. \_\_\_\_\_

iii. What is the average red:gray ratio between 300–320 rounds?

iii. \_\_\_\_\_

iv. What do you predict will be the average red:gray ratio between 10000–12000 rounds?

iv. \_\_\_\_\_

v. Look at the graph (upper panel). When does the graph (of bulk concentration) “stop changing”?

v. \_\_\_\_\_

vi. Look at the individual dice (lower panel). When does the individual dice stop changing?

vi. \_\_\_\_\_

vii. What have you learnt about a system at equilibrium?

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2. Starting conditions

(a) Run a simulation with the following conditions: dieCount = 500, **initial remain = 500**, dieSide = 100, forwardConditions = 30, backwardConditions = 10, mystery = 500. What is the equilibrium red:gray ratio?

(a) \_\_\_\_\_

(b) Run a simulation with the following conditions: dieCount = 500, **initial remain = 250**, dieSide = 100, forwardConditions = 30, backwardConditions = 10, mystery = 500. What is the equilibrium red:gray ratio?

(b) \_\_\_\_\_

(c) Run a simulation with the following conditions: dieCount = 500, **initial remain = 0**, dieSide = 100, forwardConditions = 30, backwardConditions = 10, mystery = 500. What is the equilibrium red:gray ratio?

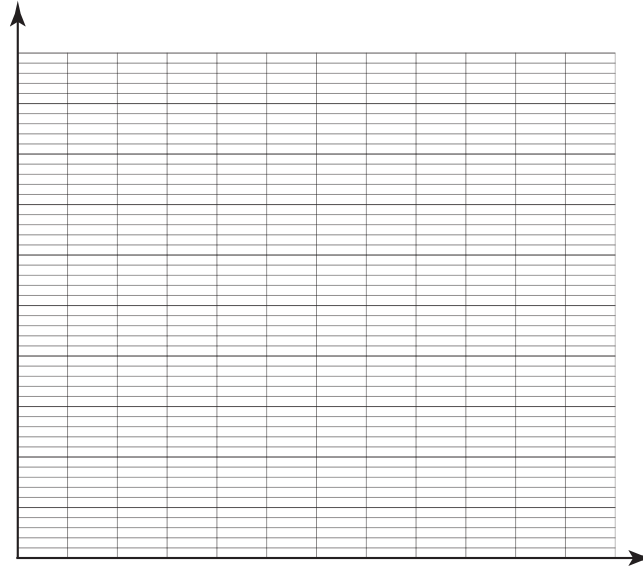
(c) \_\_\_\_\_

(d) How does the equilibrium red:gray ratio depend on the initial conditions?

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### 3. Leakage

Run a simulation with the following conditions: dieCount = 500, initialRemain = 500, dieSide = 100, forwardConditions = 30, backwardConditions = 10, mystery = 500. Let this run to 300 rounds and pause the simulation.



- (a) Sketch a graph of the simulation.
- (b) Imagine that each round we remove five dice. Sketch how this would affect the simulation.
- (c) At which round would an equilibrium be established?

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- (d) What have you learnt about the prerequisite of an equilibrium?

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4. Rates ratio and product ratio

Starting with dieCount = 1000, initial remain = 1000, dieSide = 100, mystery = 500.

- (a) Keeping backwardConditions = 10, run a series of simulations with forwardConditions at 2, 5, 10, 20, 30. Let these systems to come to an equilibrium, and tabulate your data.

Table 1 Record of rate simulation

Expt	Forward	Backward	F:B ratio	Eqm red:gray ratio
1	2	10		
2	5	10		
3	10	10		
4	20	10		
5	30	10		
6	50	10		

- (b) What is the relationship between forward/backward conditions and the equilibrium red:gray ratio? Give evidence to support your claims.

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5. Rates and product ratio

Starting with dieCount = 1000, initial remain = 1000, dieSide = 100, mystery = 500.

- (a) Run a series of simulations with the following conditions. Let these systems to come to an equilibrium, and tabulate your data.

Table 2 Record of rate simulation

Expt	Forward	Backward	F:B ratio	Eqm red:gray ratio
1	2	2		
2	3	3		
3	4	4		
4	10	10		
5	20	20		

- (b) If we keep the forward:backward ratio constant, but change their magnitude, how does this affect the equilibrium red:gray ratio? Give evidence to support your claims.

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- (c) A catalyst increases the rate of both the forward and backward reactions. How would it change the equilibrium ratio of the products?

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