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ALGORITHMS AND THEIR APPLICATION IN CHEMISTRY

Abstract. *The article examines how chemical processes and problems can be modeled algorithmically using algorithms, which are applied to applied mathematics, in particular to chemical processes, and their significance is revealed.*

Keywords: *algorithm, sequence, chemistry, chemical processes, iterative, branching, linear, modular algorithms modeling, number of moles, molar mass, temperature.*

Algorithm By "routine" is usually meant a set of precise, sequential, and repeatable operations. Algorithms in higher mathematics are essentially structured this way. They are a set of steps designed to solve a specific mathematical problem, each step of which is clearly defined.

We will look at the types of algorithms and their applications to chemistry.

1. Linear algorithm (sequential algorithm)

▶ Definition:In the algorithm, all operations are performed sequentially, there is no branching or repetition.

✅ Features:

• Each step is performed in a specific order.

• There are no conditions.

Application of linear algorithms in chemistry.

Issue: Calculate how many grams of a substance is equal to 1 mole.

Formula: mass = number of moles × molar mass

This calculation is performed sequentially, i.e. it is an example of a linear algorithm.

Steps of the algorithm (in linear form):

1) Enter molar mass (M)
2) Enter the number of moles (n)
3) Mass calculation: m = n × M
4) Output

Example: How many grams are 2 moles of water (H_2 O)?

Solution:

1) Molar mass (H2O)

H=1*2=2 g/mol

O=16 g/mol

General: M=18 g/mol

2) Number of moles

n=2 moles

3) Calculation

m=n*M=2*18=36 grams

Conclusion: In this calculation, all operations were performed sequentially, there were no conditions or repetitions — so this is a linear algorithm.

2. Iterative algorithm (iterative algorithm)

▶ Definition:In an algorithm, an action or group of actions is repeated a number of times. The number of repetitions is predetermined or determined by a condition.

✅Features:

• There will be loops in the form of "For", "While" or "Repeat...Until".

Application of iterative algorithms in chemistry.

Problem: During the experiment, the temperature increases by 2°C every 5 minutes. If the initial temperature is 20°C, calculate how the temperature changes over 1 hour.

In this problem, the temperature increases every 5 minutes, meaning that one action is repeated continuously — this is a recursive algorithm.

Algorithm steps:

1) Setting the initial temperature:

T = 20°C

2) Starting time at 0:

t = 0

3) Recurring action (1 hour = 60 minutes, every 5 minutes):

- Every time T = T + 2
- t = t + 5

4) Output the result at each stage (optional)

5) Repeat: until the time reaches 60 minutes

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Vaqt (daq.)	Harorat (°C)
0	20
5	22
10	24
15	26
...	...
60	44

> **1 soat oxirida harorat: 44°C**

Conclusion: In this problem, the same action (increasing the temperature by 2°C) is repeated every 5 minutes — this is an example of a classic iterative algorithm.

3. Branching algorithm (conditional algorithm)

▶Definition:In an algorithm, a path is chosen based on a condition (if-else).

✅Features:

- The decision is made.
- Different paths are chosen in different situations.

Application of branching (conditional) algorithm in chemistry.

Issue: Determining the physical state of matter.

Condition: The temperature of the water is given. Depending on it:

- If the temperature is < 0°C — ice (solid)
- If 0°C ≤ temperature < 100°C — liquid
- If the temperature is ≥ 100°C — steam (gas)

Here, there are conditions and different paths are chosen based on them — this is a clear example of a branching algorithm.

Algorithm steps:

1) Enter the temperature value (T)

2) Check the condition:

- If T < 0 → "Physical state: Ice (solid)"
- Otherwise if T < 100 → "Physical state: Liquid"
- Otherwise → "Physical state: Vapor (gas)"

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25	Suyuqlik
100	Bug' (gaz)

Conclusion: In this case, conditional decisions are being made depending on the temperature. The result changes depending on the condition. So this is a branching (conditional) algorithm.

4. Recursive algorithm (self-calling)

▶ Definition: The algorithm calls itself to execute a smaller version of itself. Each call brings the result closer to the final state.

✓ Features:

- Each time it calls itself with a smaller subproblem.
- Once it reaches the base position, it begins to return.

Application of recursive algorithm in chemistry.

Issue: To understand the levels of chemical elements, calculate the number of electron shells from the number of protons (in a simple model).

A simple rule-based model (for understanding):

Let's assume that the electrons are arranged in layers as follows:

- 1st floor: 2 electrons

- 2nd layer: 8 electrons
- Layer 3: 8 electrons
- and so on...

Given the number of electrons, we recursively determine how many shells are filled.

Example: If there are 13 electrons - how many shells are filled?

For example: e = 13

- 13 > 10, so 1 + floor_number(13 - 8 = 5)
- 5 <= 10 → goes to the 2nd floor
- Result: 1 + 2 = 3 floors

Conclusion: Here, the layer_number function is repeatedly calling itself, decreasing the number of electrons. This is the simplest and most chemistry-friendly version of the recursive algorithm.

5. Modular algorithm

▶The main principle of a modular algorithm is that each module performs a separate task.

Application of modular algorithm in chemistry.

Issue: Dividing the chemical calculation process into small modules.

Example: Calculating the mass of a chemical substance.

Problem: To find the mass of a substance, we know the molar mass and the number of moles of the substance.

Modules:

1) **Molar mass calculation module**

(Finds the total molar mass by entering the atomic mass of the elements and their number)

2) **Mass calculation module**

(Mass is calculated by giving molar mass and number of moles)

3) **Output module**

Example: List of elements:

- H: 2, atomic mass 1 g/mol
- O: 1, atomic mass 16 g/mol

Number of moles: 3 moles

Calculation:

- Molar mass = (2×1) + (1×16) = 18 g/mol
- Mass = 18 × 3 = 54 grams.

Conclusion: Here, each module performs a separate task — this was the basic principle of the modular algorithm. In chemistry, dividing complex calculations into smaller parts and modules makes calculations easier.

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