ENHANCING CONCEPTUAL UNDERSTANDING OF THERMAL PARTICLE DYNAMICS AND PHASE TRANSITIONS THROUGH SIMULATION-BASED LEARNING

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ABSTRACT

This article examines the efficiency of the simulation model “Modello particellare” in the teaching of basic concepts related to the dynamics of matter and thermal particles using oxygen as a representative example. The simulation provides an interactive platform that allows students to visually and dynamically observe molecular behavior at the submicroscopic level. Illustration of phase transitions - for example, liquid and gas liquid - simulation allows students to concept of particle interactions, thermal dynamics and related phenomena more intuitively. The remarkable function includes an interactive phase diagram equipped with a dynamic brand that provides real - time feedback on temperature changes and physical condition. In addition, the simulation effectively demonstrates the irregular movement of particles caused by frequent molecular collisions, which illustrates the affordable concepts of complex concepts such as Brownian’s motion.

Keywords: Dynamics of thermal particles, phase transitions, interactive simulation, Brownian motion, submicroscopic visualization, simulation-based learning.

INTRODUCTION

Traditional approaches often do not reach and try to bridge the gap between theory and application in the real world. According to Atkins, chemistry of education bridges macroscopic observations and microscopic imagination. It emphasizes three key challenges: abstraction, mathematical problems and overall complexity. Henry (2004) argues that communication in chemistry requires strong visual strategies. This can be confused by students if they are not properly solved. To overcome them Atkins recommends, using visualization tools and simulation models to increase understanding. Free simulation tools provide tangible learning benefits (Belli et al., 2024). Visually engaging tools are considered essential for enhance students the phase transitions at the particulate level (Slapničar et al., 2020). 3D animations significantly enhance student comprehension in natural science subject.

Model description and application

The simulation tool, freely available online, was developed using HTML5, JavaScript (ES6), XML, JSON, SVG and Canvas (see Figure 1). The code describing the dynamic movement of particles is based on Brownian’s motion and simulates the balance of repulsive and attractive forces in solids, liquids and gases. In each state of matter, the movement of particles depends on the kinetic energy that corresponds to the system temperature. In liquids, attractive forces predominate over repulsive and gravity have a stronger effect compared to gases, causing the particles to settle towards the bottom of the virtual container such as a beaker. In the solids, the particles are fixed in the organized grid structure (Figure 2) that cannot move freely between the cells but capable of vibrating according to the temperature.

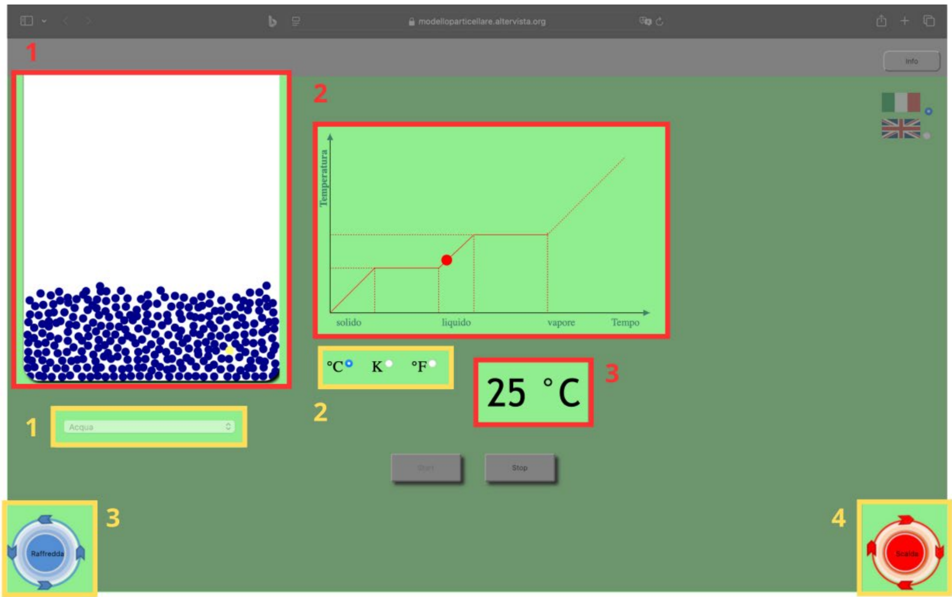


Fig.1. Molecular thermal motion experiment display

Simulation Controls (Yellow): 1. Substance Selection (for choosing different materials). 2. Temperature Unit (°C/°F/K).3. Increase Temperature. 4. Decrease Temperature.
Display Windows (Red): 1. Experiment Viewport (for the main simulation window). 2. Thermal Analysis Graph (for the graphical data display). 3. Temperature display

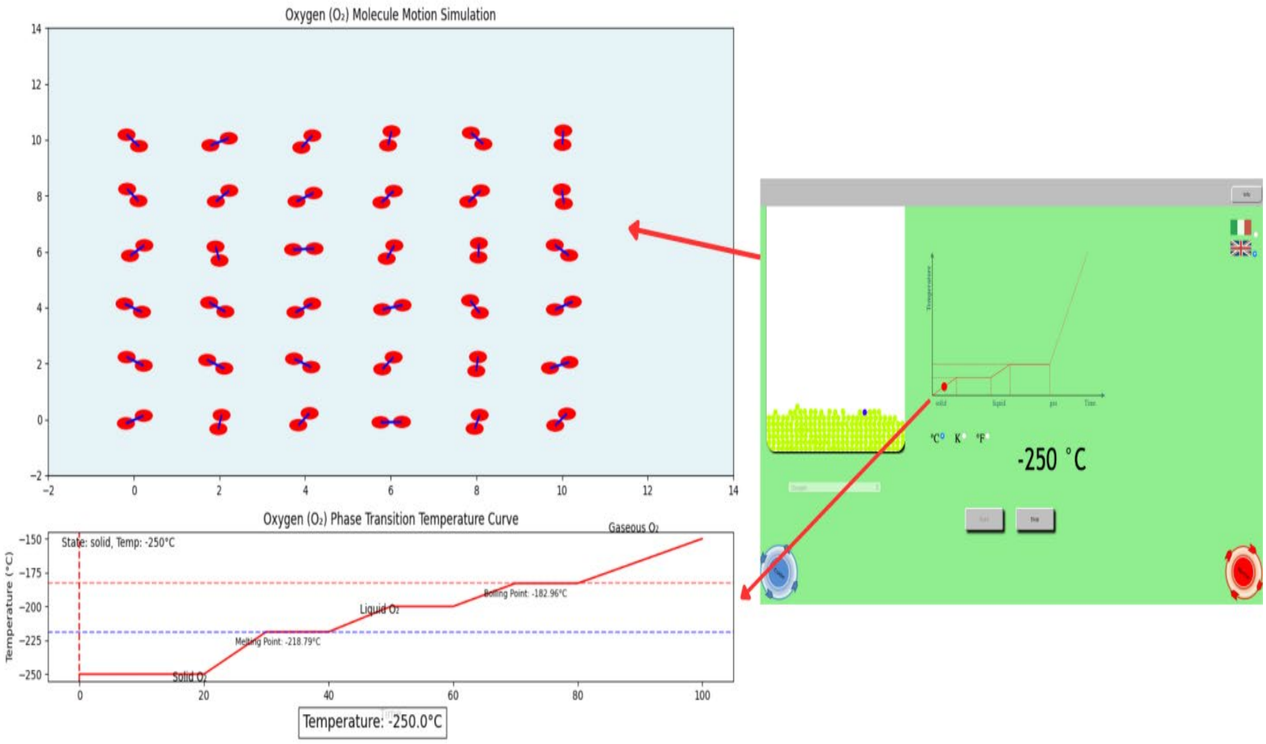


Fig.2. Simulation of molecular movement and phase transition of oxygen

The figure shows oxygen molecules in a solid phase at –250 ° C, arranged in a fixed structure, similar to the grid with a minimum movement due to strong intermolecular forces. The lower graph shows the phase transition curve for oxygen, marking its melting point (–218.79 ° C) and the boiling point (–182.96 ° C). This visual highlights how oxygen changes the phases depending on temperature.

After clicking on the link provided (http://modelloparticellare.altervista.org/), students approach a website showing an empty beaker on a green background. The language can be switched between English and Italian using the selection menu located in the upper right corner of the interface. In addition, it is located in the lower left corner of the drop-down menu, from which students can choose specific substances, namely water, molecular oxygen, table salt and tert-Butyl alcohol (see Figure 3). After selecting the fabric and pressing the "Start" button, the beaker, originally empty, fills the animated particles in motion. These particles visually represent a thermodynamically stable condition of the selected substance at 25 °C at atmospheric pressure. As illustrated by images in Figure 3, four selected substances were deliberately chosen because of the fact that three of them - water, sodium chloride and molecular oxygen - are known materials that naturally exist in different physical conditions at room temperature. The fourth substance does not normally fit in everyday life; However, it has a significant value due to its phase transition with fixed liquids, which occurs to the approaching room temperature. Thanks to this characteristic, it is particularly suitable for a safe and effective demonstration of melting and solidification processes. An important aspect of the simulation tool is its interactive phase diagram with a dynamic red marker, which continuously reflects the temperature in real time and corresponding to the physical condition of the substance. At the bottom of the interface are two interactive controls - one red for heating and one blue for cooling - which students can alternately use to virtually modify the sample temperature. The software immediately responds to these changes and corresponds appropriately to the visual representation in the beaker and the phase diagram. In addition, they have the opportunity to switch between different temperature units, including Celsius, Kelvin and Fahrenheit.

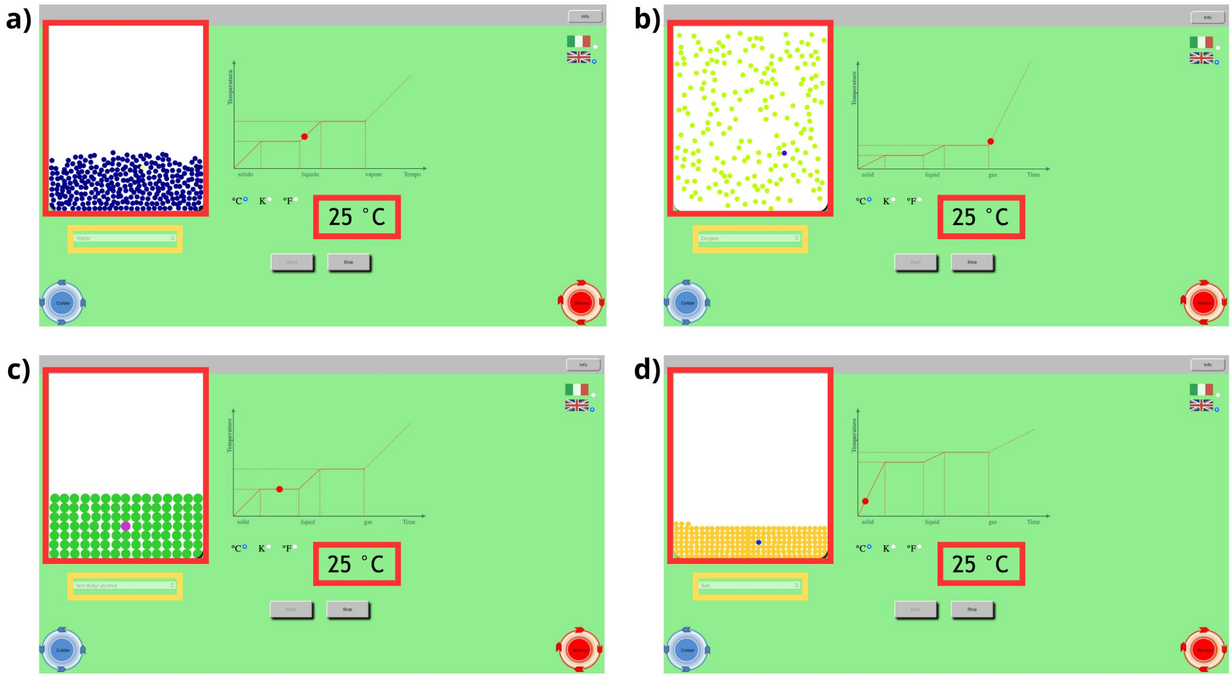
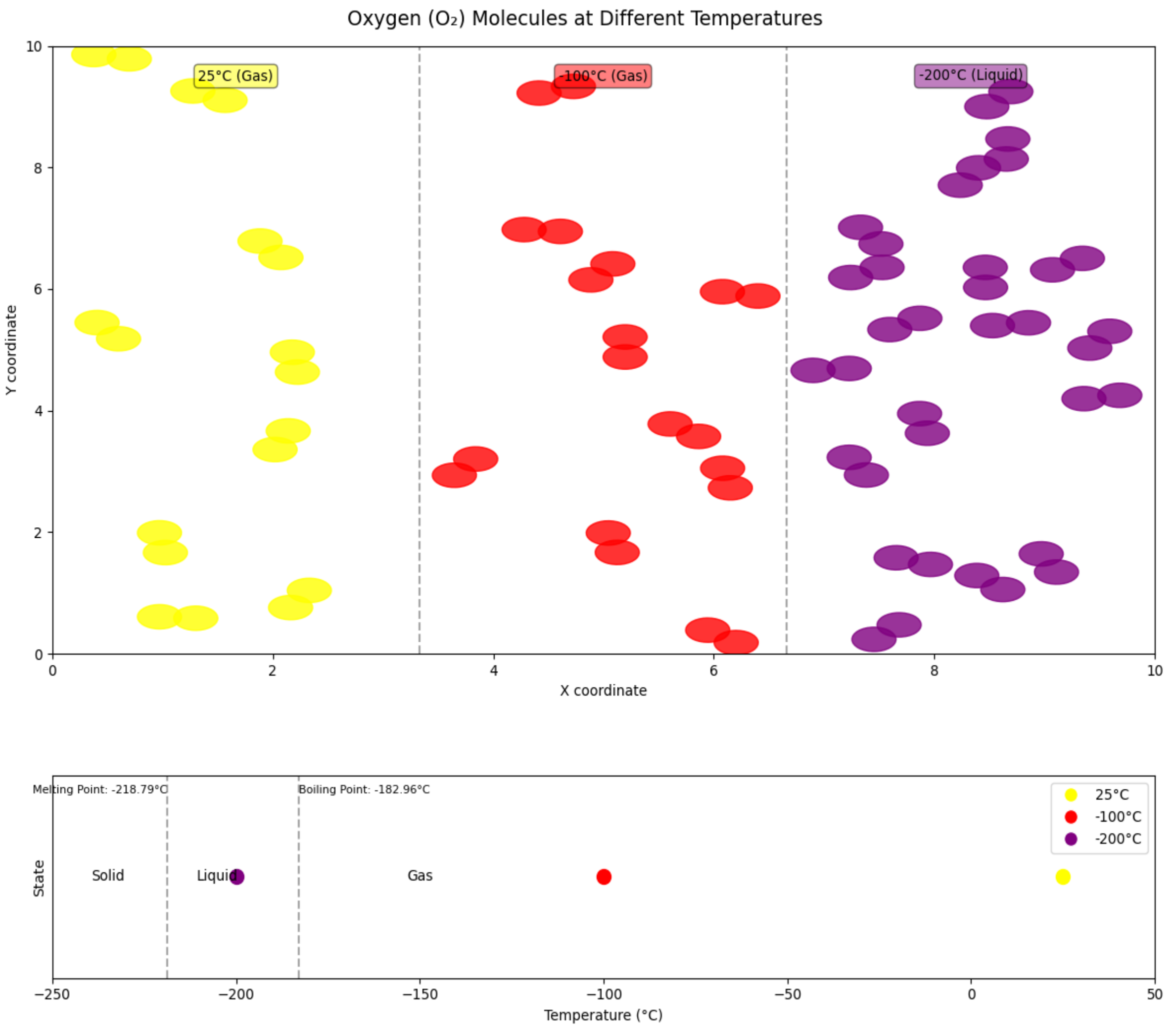


Figure 3. Simulation of different substances in different states at room temperature (25 °C)
This figure has the simulation of four substances at 25 ° C: (a) water, (b) oxygen, (c) third-butyl alcohol and (d) salt. Each subfigure shows a molecular (left) and a corresponding temperature graph (right). Water molecules appear very full but mobile, indicating a liquid state. Oxygen molecules are widely scattered and quickly, which represents a gas. Alcohol and third-butyl salt exhibit fixed and orderly network structures, characteristics of solids at room temperature.

The increase in temperature to 100 ° C (373 K) maintains oxygen in gaseous state, as 100 ° C remains significantly above the boiling point of –183 ° C. However, these temperature increases significantly change the behavior of molecules. From the point of view of Brownian's motion, the random movement of oxygen molecules at 100 ° C becomes more energetic and more prominent. The



intensity of Brownian's motion is directly related to the temperature; As the temperature increases, the chaotic thermal movement of the particles is intensified. At 100 °C, the simulation clearly shows that oxygen molecules move faster and in more unpredictable trajectories.

Fig.4. Oxygen molecules arrangement at different temperatures

This figure illustrates the molecular behavior of oxygen (O_2) at three temperatures: 25 ° C (yellow, gas), –100 ° C (red, gas) and –200 ° C (purple, liquid). The upper panel shows the distribution of particles and proximity, while the lower panel has a phase diagram that indicates the fusion of oxygen (–218.79 ° C) and the boiling points (–182.96 ° C). At 25 ° C, the molecules are widely spaced and highly mobile, which reflects high kinetic energy. A –100 ° C, they remain softly but move less and are more compact. A –200 ° C, the molecules are grouped densely with a minimum movement, indicating liquefaction.

Unlike intense winding movements observed at 25 °C or 100 °C, the movements at –200 °C are highly limited and slow, as the molecules lose freedom of movement due to narrowly surrounded particles. This clearly shows the temperature dependence of Brownian's motion: as the temperature decreases, the molecular kinetic energy decreases, which significantly slows down random molecular movements. When the oxygen approaches the firm state, the molecules are limited to vibrations around solid positions, causing Brownian's motion almost disappear.

DISCUSSION

The "Modello Particellare" simulation presents a range of pedagogical advantages that make it a valuable tool to teach dynamics of thermal particles and phase transitions. One of its key strengths is found in its visual and interactive nature, which allows students to observe the molecular movement in real time. This facilitates a deeper conceptual understanding of the behavior of particles at the submicroscopic level (Belli et al., 2024; Teplá et al., 2022).

The model also unites the gap between abstract theory and observable phenomena, reinforcing key scientific concepts such as diffusion, condensation and Brownian motion (Tang and Abraham, 2016).

Another benefit of simulation is its versatility through educational levels. Whether it is used in high school or undergraduate environments, it can be adapted to coincide with the previous knowledge of the student, so it is an accessible teaching assistance (Reina et al., 2024).

Particle-based simulations are aligned with constructivist learning theories by allowing students to actively build understanding through visual research and manipulation (Wu and Shah, 2004). Interactive models help reveal and correct alternative conceptions, especially when students make predictions and try them in real-time environments (Treagust et al., 2011). When used beyond contexts in the classroom, such simulations can promote autonomous learning and promote a deeper commitment to chemical phenomena (Chiu and Lin, 2005).

CONCLUSION

This technology message is an interactive software tool with an open-source code developed to introduce the particle model. The software helps students to understand what is happening at a submicroscopic level when the substance passes from one condition to another (for example, from solid to liquid and vice versa or from liquid to gas and vice versa). This digital tool can effectively introduce students to the simplest model of particles of matter without required to require previous knowledge of atoms, molecules or ions. The interactive functions of the software facilitate the understanding of the thermal particle dynamics and how the particle movement is related to the temperature. This particular aspect is difficult to understand without using the dynamic model. The proposed software has proven to be particularly effective in illustrating, interactively and clearly, submicroscopic and thermal transformations using oxygen as an example and their relationship to Brownian motion.

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