Liite 2

MoTc Animation Design Research

Edumendo - Advanced Learning and Visualization Research

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Project details:

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Edumendo – Advanced Learning and Visualization Oy is a unique design company that applies modern learning and psychological theories in mathematical and natural science domains. Edumendo provides special tailored and highly sophisticated visualizations and high level consultation services for marketing, client- vendor interaction and personnel’s professional growth purposes.

Content

1. Introduction

This report describes an animation project, which goal was to create a research-based chemistry animation that visualizes the decay of molybdate (MoO_4^{2-}) to pertechnetate (TcO_4^-) and TcO_4^- elution process that includes water molecules (H_2O), sodium ions (Na^+) and chloride ions (Cl^-) (CD-ROM).

The goals of this report are:

- to document the MoTc animation design research project to the vendor and to the customer,
- to provide more resources to the customer for using the animation and
- to illustrate possibilities and challenges of the project so that in the future it is possible to achieve a higher level of a consensus and improve design in general.

The animation was produced using a Model-Based Design Research approach [1]. The reliability of the animation was confirmed by using a chemistry expert in the visualization design and a model based consensus building between the vendor and the customer. The created animation is also a teaching model with several limitations which are explained in this research report (see chapter 4.2.1).

A Model-Based Design Research [1] is a cyclic process, including every phase of a design research: i) design procedure (see chapter 2), ii) problem analysis and iii) design solution (see chapters 3 & 4) [2]. Design processes are carried out through a change of an ontological status of a model concept [3]. In order to achieve an exquisite level of consensus on the MoTc animation teaching model, the design project was divided into three phases:

1. Initial meeting,
2. Design solution I: Storyboard (see chapter 3) and
3. Design solution II: MoTc animation (see chapter 4).

For full understanding of the consensus building process of this research, it is important to explore some to some theoretical issues related to chemistry animations (see chapter 1.1) and to get to know the ontological changes of a model concept (see chapter 1.2).

1.1 Introduction to chemistry animations

Animations are powerful tools for visualizing sub-microscopic changes and they promote understanding of complex chemical concepts [4]. According to research literature, observing animations improve students' ability to sketch connections between macro, symbolic and sub-microscopic levels and develop their mental models more dynamic. It is also presented that one of animations major benefits in chemistry education is that it enables people to discuss chemistry on a molecular level [5,6].

Animations are not interactive and they do not base on real data. Animations represent purely a modellers' mental model and are sensitive to graphical expression skills, which makes creating good and pedagogically meaningful animations a challenging task. Meaningful chemistry animations are i) short, illustrating one concept under 60 seconds, ii) understanding is supported through voice or text narration, iii) the user interface is clear, iv) the content is tested with students and experts and v) it also is important to plan the design process based on research literature. [7]

1.2 An ontological status of a model concept

Models and modelling are essential tools and a way of thinking in chemistry. Models can be e.g. pictures, gestures, chemical symbols, mathematical symbols, graphs, maps or animations and they can be made by using gestures, pencil and paper, thoughts or computers, for example. Chemists use models in every phase of modern chemistry. For instance, they are used as tools for making hypothesis, explanations, representations of processes, phenomenon and results. Indeed, models serve as links between theoretical and practical chemistry and they are constructed for a specific purpose. [3]

An ontological classification of models is possible to carry out by studying different variations of models (see figure 1). When a model is a personal and private representation of a certain phenomena, it is called a mental model. The mental model changes into an expressed model after it is published in a group or a public domain. When different social groups interact and test the expressed model and come to an agreement of the purpose and characteristics of it, the expressed model becomes a consensus model. The consensus model can be a scientific model, if consensus is formed by a community of scientists, or a historical model, if it has a historical purpose, for example. Historical and scientific models are often complex and difficult to understand. In order to make the understanding easier, teachers and students build teaching models to assist learning, e.g. a computer constructed animation with educational purposes. [3]

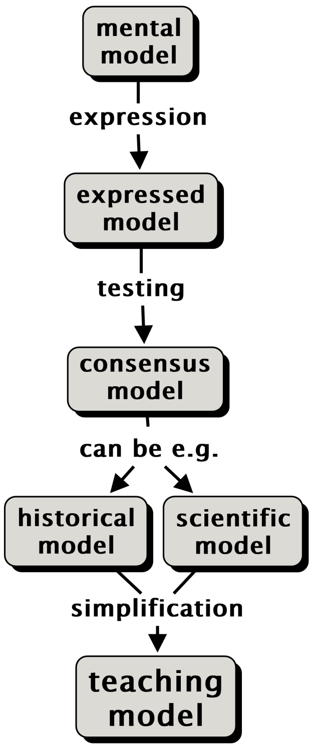

Figure 1. *An ontological classification of models*

2. Design procedure

This design research included three phases (see figure 2):

1) Initial meeting

The research project started with an initial meeting in Helsinki in 4th June where the goals of the project and project time lines were agreed and some preliminary sketches were illustrated.

2) Design solution I: Storyboard (see chapter 3)

After the initial meeting, a storyboard phase started. The storyboard phase included two parts: problem analysis 1 and consensus model 1.

In the consensus model 1 phase, vendor's animator and chemistry expert built the first consensus model of the animation. The modelling process in consensus model 1 part was: animator's mental model → expressed model → consensus model (see figure 1).

The storyboard was sent to the customer in 16th July.

3) Design solution II: MoTc animation (see chapter 4)

MoTc animation phase included two parts: Problem analysis 2 and consensus model 2. In the problem analysis 2, the feedback from the customer was analysed resulting in a few changes to the animation. In the consensus model 2 part, the animation had achieved a consensus between the vendor and the customer and the final renderings were carried out.

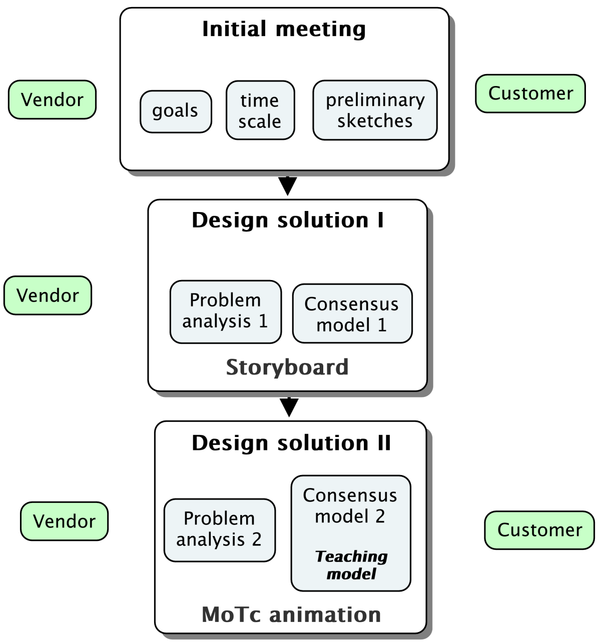

Figure 2. *Design research procedure*

3. Design solution I: Storyboard

The storyboard phase visualized the consensus model 1 of the MoTc animation. The objective of the storyboard was to publish the current consensus model to the customer, so that the customer could analyze it and give feedback to the vendor.

The storyboard included:

1. Problem analysis 1 (3.1)
    - A summary of the chemistry of ^{99m}Tc Generator prepared by radio chemist (3.1.1)
    - A study of earlier visualizations (3.1.2)
    - A study of Blender 3D (3.1.3)
2. MoTc animation presented via still images, including chemistry and visualization explanations (3.2)
3. Technical details of the storyboard animation (3.3)
4. A low resolution demo rendering (CD-ROM)

3.1 Problem analysis 1

The goal of the problem analysis was to reveal the possibilities and challenges of the animation.

3.1.1 Chemistry of the ^{99}Mo/^{99m}Tc generator

Molybdenum-99 – Technetium-99m -generators are the most widely used radionuclide generators in the world. The advantages of the ^{99}Mo/^{99m}Tc generator are mostly due the physical properties of the daughter nuclide, metastable technetium ^{99m}Tc. The element technetium has seven different possible valence states, giving it unparalleled chemical versatility when considering radio labeling. ^{99m}Tc has a short half-life, 6 hours, in terms of metabolism and it emits single, easily detectable 140 keV gamma ray which makes it ideal radionuclide for diagnostic purposes. [8,9,10].

^{99m}Tc is produced inside the generator from the decay of ^{99}Mo by the following process (figure 3):

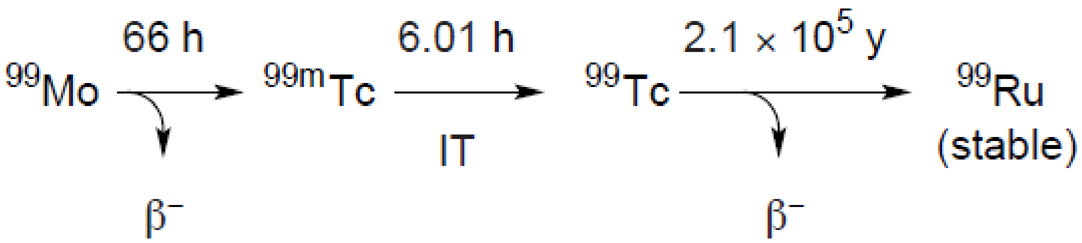

Figure 3. Decay scheme of molybdenum-99

Inside the generator, ^{99}Mo is adsorbed onto alumina (Al_2O_3) as molybdate, MoO_4^{2-}. Molybdenum in molybdate decays to technetium, forming a pertechnetate ion TcO_4^-, which because of its single charge is less tightly bound to the alumina than the molybdate [11].

The pertechnetate ion formed can then be easily eluted from the generator using a solution containing an electrolyte, most commonly aqueous 0.9 % sodium chloride:

$$^{99}MoO_4^{2-} + 2X^+ \xrightarrow{\beta^-} X_2{}^{99}MoO_4 \longrightarrow X^+ + X^{99m}TcO_4$$

$$X^{99m}TcO_4 + NaCl \longrightarrow XCl + Na^{99m}TcO_4$$

where X is the monovalent binding site on alumina inside the column.

As presented above, elution with sodium chloride replaces the $^{99m}TcO4^-$ with Cl^-. This removes all of the ^{99m}Tc from the generator but leaves the $^{99}MoO_4^{2-}$on the alumina column. More ^{99m}Tc will then regenerate from the parent nuclide.

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3.1.2 A study of earlier visualizations

Suitable animations for this topic were studied in order to study how similar phenomenon has been visualized before; what are limitations of these visualizations and what challenges there might be? Altogether nine animations were analyzed (see table 1).

Table 1. *Earlier beta and gamma radiation animations*

#	Beta radiation	Gamma radiation	References (26.9.2010)
1	Blue particles moving faster than alpha radiation particles	Fast lighting arrow	Furry Elephant physics: http://www.furryelephant.com/player.php?subject=physics&jumpTo=re/2Ms4
2	Green particle	Yellow arrow	Radiation Emergency Medical Management (REMM): http://www.remm.nlm.gov/beta_animation.htm
3	Particle	Orange arrow	http://www.newcastle-schools.org.uk/nsn/chemistry/radioactivity/Three%20Types%20of%20Radiation%20Page.htm
4	Light blue particle and properties	Arrow and properties	Wikipedia: http://en.wikipedia.org/wiki/File:Alfa_beta_gamma_radiation.svg
5	Purple particles	Four yellow arrows at the same time and rotating system, black background, animation length 41 seconds	You tube, Radioactive decay animation: http://www.youtube.com/watch?v=crtTQOeUJYU&feature=related
6	Voice narration and rotating system		You tube, Radioactive decay document: http://www.youtube.com/watch?v=EiYYi-QGddE&feature=related
7	Voice narration, black background, explosion visualization		You Tube, Nuclear physics in 3D: http://www.youtube.com/watch?v=aldk-HWESzw&feature=related
8	Single fast flash with a light tale	Yellow arrow, space background, length 34 seconds	You Tube, Atomic decay: http://www.youtube.com/watch?v=Ks5OB7e-M24&feature=related
9	Purple or green particles	Yellow arrows, black background	You Tube, Nucleus animation: http://www.youtube.com/watch?v=BfBI_4WqVEU&feature=related

This visualization study revealed that this field only had a few earlier visualizations. Some of the studied visualizations were poor quality and models extremely simplified. Earlier visualizations were also repetitive. Beta radiation was always visualized using solid particles and gamma radiation using arrows. Only solid aspects of the earlier animations were a voice narration in some visualizations and a black background.

According to this study, the main challenges of this animation design research was, that what is a new way to visualize beta and gamma radiation and also make it look scientifically meaningful.

3.1.3 A study of Blender 3D

Blender 3D is an animation software, which offers new ways to visualize chemistry. Blender is used in film making and provides more diverse visualization resources than regular chemistry animation software (see figure 4). Edumendo company has designed a software that allows to import molecule coordinate data inside the Blender, which gives the needed advantage to earlier visualizations of this field.

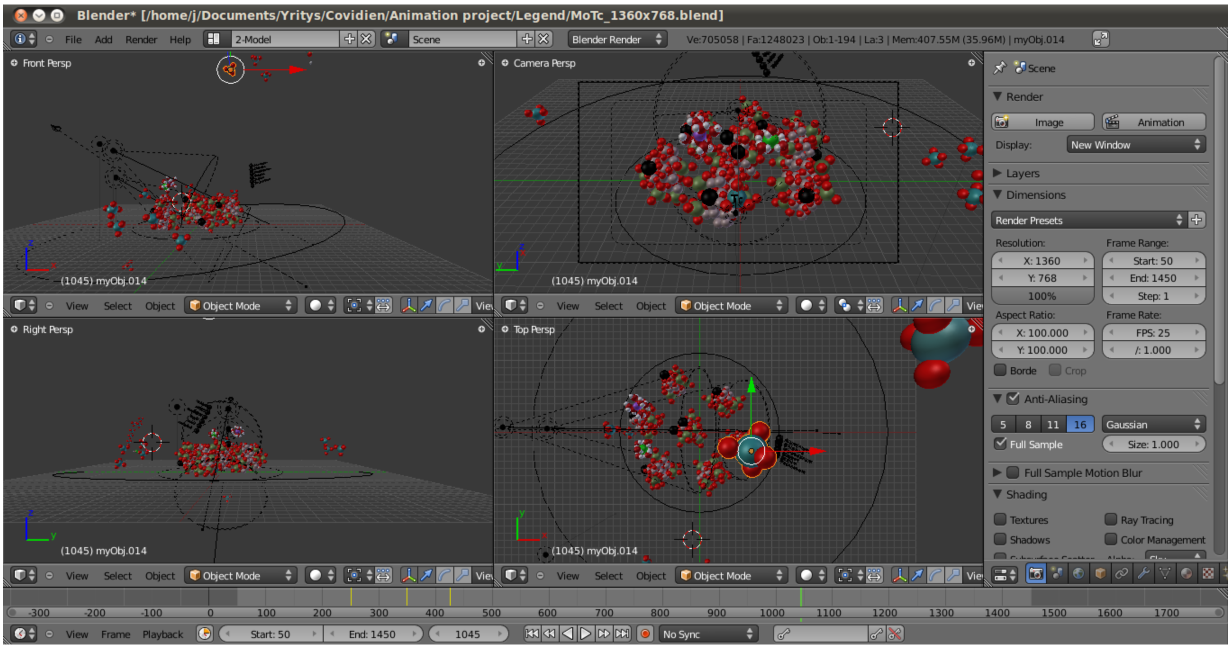


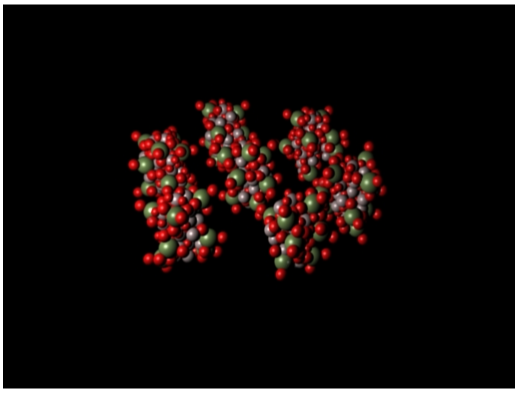
Figure 4. *Blender 3D user interface*

After studying Blender properties, beta and gamma radiations were produced using Blender particle effects. This way it was possible to make the gamma radiation look like a controlled impulse that is used safely in the drug that the MoTc generator produces and to avoid the regular arrow type of visualization.

Beta particles were made transparent and not solid like in the earlier visualizations. The main idea was to build controlled gamma flashes from the multiple beta particles in order to illustrate the change that happens in the generator.

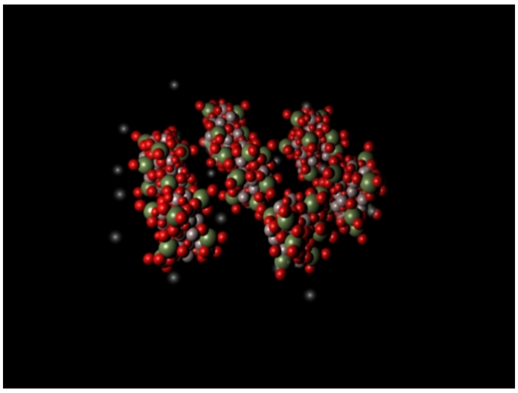
3.2 Consensus model 1: 99Mo / 99mTc animation via still images

This animation is a simplified description of a chemistry of $^{99}Mo/^{99m}Tc$ generator. As 87, 5 % of molybdenum decays straight to ^{99m}Tc, decay of molybdenum to long lived ^{99}Tc has been excluded from this animation. In the modeling, cpk-molecule model has been used, because it illustrates the adsorption more accurately than other molecule models (e.g. wireframe, wire, ball & stick) (see figures 5-14).



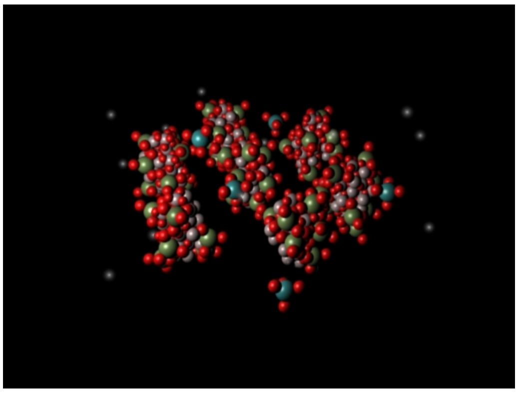
Chemistry: ^{99}Mo is adsorbed onto the alumina as molybdate $^{99}MoO_4^{2-}$ [8].
Visualization: Camera captures the full overview.
- 7 Al_2O_3 pillars
- about 50 $^{99}MoO_4^{2-}$

Figure 5. *Scene 1 (start) (1st frame of the animation)*



Chemistry: ^{99}Mo emits beta particles.
Visualization: Camera captures the full overview.
- Animation contains 11 different kind of beta particle emitters.
- Beta particles are emitted through animation.

Figure 6. *Scene 1 (middle)*



Chemistry: ^{99}Mo decays to ^{99m}Tc forming pertechnetate ion $^{99m}TcO_4^-$, which is less tightly bound to the alumina than molybdate [8,11].
Visualization: Camera captures the full overview.

Figure 7. *Scene 1 (end) & Scene 2 (start)*

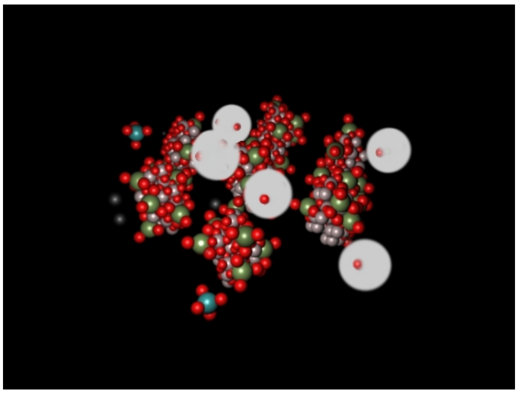


Figure 8. *Scene 2 (middle)*

Chemistry: ^{99m}Tc emits 140 keV gamma rays.
Visualization: Camera rotates 90 degrees to the left in order to visualize the 3D.

- *We strongly advice to include these gamma ray visualizations in the animation.*
  → they are the safe medical used product

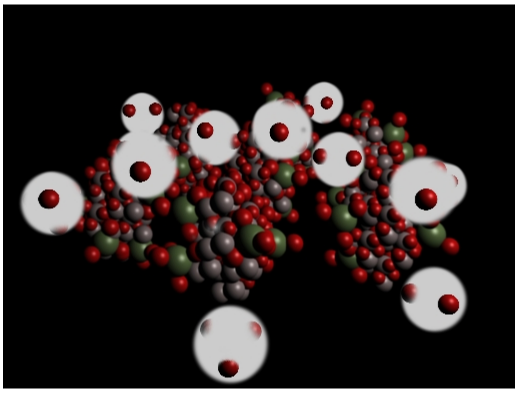


Figure 9. *Scene 3 (middle)*

Chemistry: More technetium has grown in from ^{99}Mo.
Visualization: Camera zooms in.

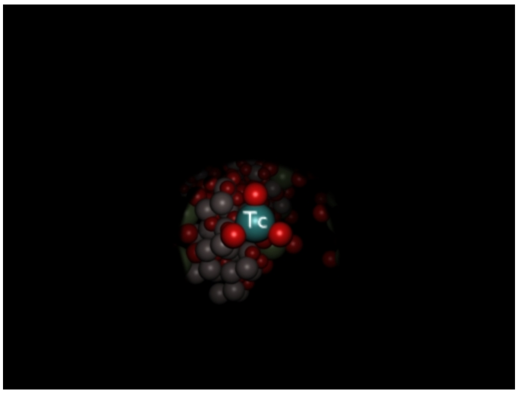


Figure 10: *Scene 3 (middle)*

Chemistry: ^{99}Mo decays to ^{99m}Tc forming pertechnetate ion $^{99m}TcO_4^-$.
Visualization: The change is emphasized by using spotlight.

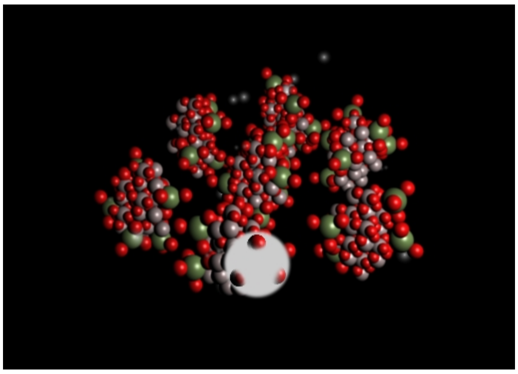
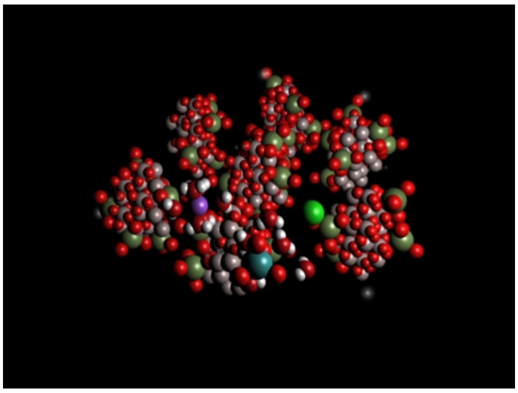


Figure 11. *Scene 4 (end)*

Chemistry: Gamma radiation
Visualization: Camera zooms out.

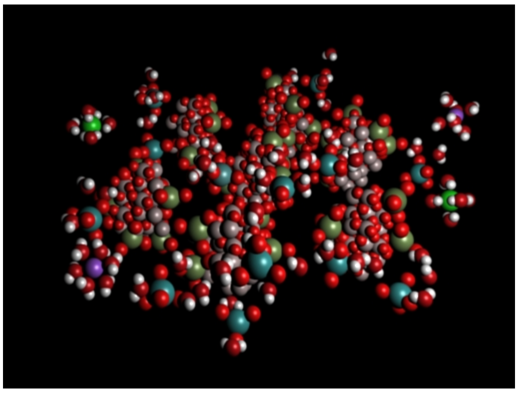
- Only one TcO_4^- ion is left. The rest of the ions have vanished during the spotlight phase in the scene 3.

  → This is done because otherwise the scene 5 (elution and ion exchange) would contain too many moving objects at the same time and would be unpleasant to watch (see figures 12 & 13).



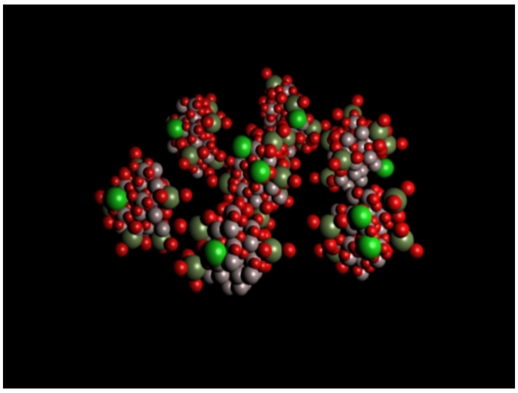
Chemistry: Elution with NaCl replaces the weakly bound $^{99m}TcO4^{-}$ with Cl^{-} and sodium pertechnetate $Na^{99m}TcO_4$ is formed. Alumina acts like an ion exchanger, releasing the pertechnetate ion and adsorbing the chloride from sodium chloride.
Visualization: Camera captures the full overview.

Figure 12. *Scene 5 (middle)*



- *Absolutely too much movement at the same time.*
- *if carried out one at the time, the animation length exceeds 60 seconds* [7].

Figure 13. *Scene 5 (alternative 2)*



Chemistry: Alumina acts like an ion exchanger, releasing pertechnetate ion and adsorbing the chloride from sodium chloride.
Visualization: Camera captures the full overview.

Figure 14. *Scene 5 (end) (last frame of the animation)*

3.3 Technical details of the storyboard animation

- Length: 52 seconds
- 1300 frames
- 25 frames / second
- File format: .avi (xvid)
- 5 scenes
    1. Start and overview (0-10 seconds)
    2. Rotation (11-15 seconds)
    3. Zoom in (16-28 seconds)
    4. Zoom out (29-33 seconds)
    5. Elution and ion exchange (34-52 seconds)
- beta particle emitters (15 – 20 particles / emitter, life: 12 frames)
- 8 gamma ray flashes (1000 particles, life: 13 frames)
- Background: black

4. Design solution II: MoTc animation

Design solution II includes two parts: Problem analysis 2 (see chapter 4.1) and consensus model 2 (see chapter 4.2).

4.1 Problem analysis 2: Customer feedback

After examining the storyboard, the customer wanted three modifications and further designs to the final version of the animation:

1. A legend that illustrates atom colours (see figure 15).
2. Darkened background to the elution scene in order to emphasize the NaCl flow (see figure 16).
3. Two versions of subtitles, a short and a long version for the needs of different kind of audiences.

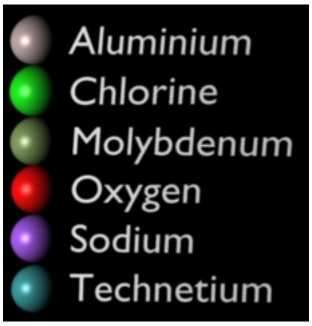


Figure 15. *Legend*

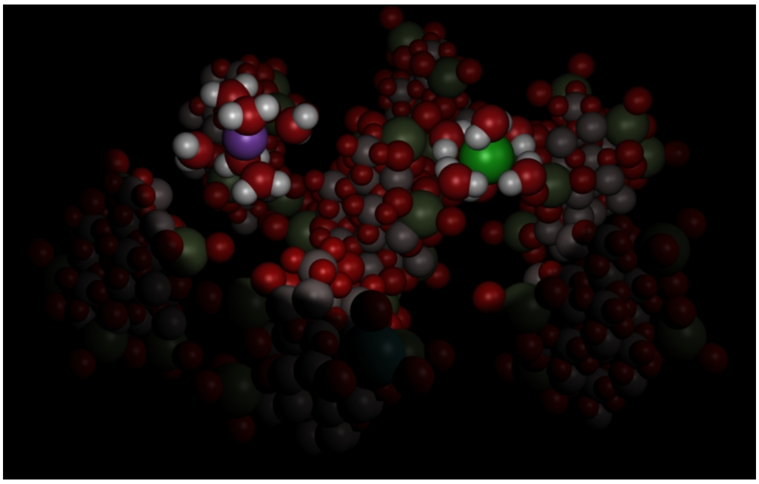


Figure 16. *Darkened background in the elution scene.*

After seeing the storyboard version, the customer also wanted to see how other background colours work. Orange and different kind of blue backgrounds were tested, but in consensus between the vendor and the customer, the black colour was kept (see figures 17 & 18).

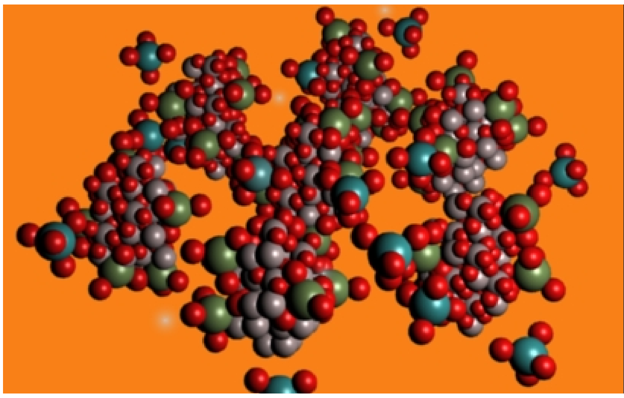


Figure 17. Orange background

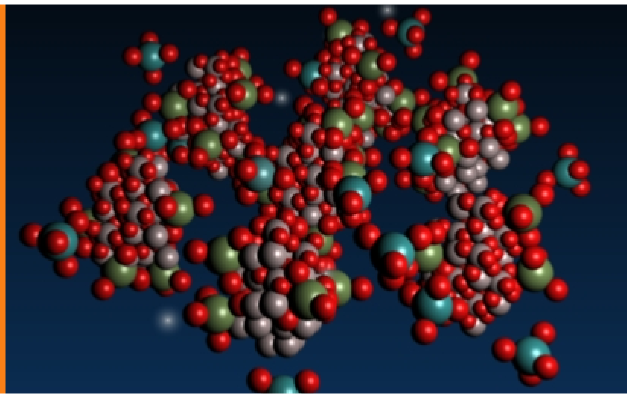


Figure 18. Gradient dark blue background

Two versions of subtitles were also produced (see table 2). The subtitle narration and legend forced a few changes to the final version of the MoTc animation in order to secure the fluent subtitle and narration flow:

- Two gamma flashes were taken out,
- the length of the start scene was increased by two seconds and
- at the end of the animation a whole new end scene was created.

These changes increased the animation length four seconds (see table 3).

Table 2. *Comparison between short and long subtitles*

Time	Short	Long
0,5 – 4,5 seconds	-	Molybdenum is adsorbed onto the alumina as molybdate
5,0 – 13,0 seconds	Molybdate ions emit beta particles and decay to pertechnetate ions	Molybdate ions emit beta particles and decay to pertechnetate ions
13,0 – 21,0 seconds (S) 13,0 – 20,0 seconds (L)	Pertechnetate ions emit gamma rays	Pertechnetate ions emit gamma rays
22,0 – 28,0	-	Pertechnetate is less tightly bound to the alumina than molybdate
36,5 – 45,9 seconds (S) 36,0 – 42,0 seconds (L)	Elution with NaCl replaces the weakly bound pertechnetate	Elution with NaCl replaces the weakly bound pertechetate with chloride and sodium pertechnetate is formed
45,9 – 49,9 seconds	Aluminium oxide acts like an ion exchanger adsorbing the chloride	Aluminium oxide acts like an ion exchanger adsorbing the chloride
49,9 – 53,9 seconds	and releasing the pertechnetate ion	and releasing the pertechnetate ion

4.2 Consensus model 2: Final version of the animation

After the changes from the problem analysis 2, the level of consensus between the vendor and the customer was sufficient and the rendering of the final teaching consensus model could get started.

In the rendering phase, seven different resolutions were rendered. The animation can be played on full screen mode with maximum performance in the most common monitors. The rendered resolutions are:

1. 640 x 480, pixels, size: 9,9 MB
2. 800 x 600, pixels, size: 12,3 MB
3. 1280 x 768 pixels, size: 16,2 MB
4. 1360 x 768, pixels, size: 18,8 MB → (this size is the most suitable resolution for the trade fair booth in 9.10.2010)
5. 1280 x 1024, pixels, size: 22,9 MB
6. 1440 x 900, pixels, size: 21,7 MB
7. 1920 x 1080, pixels, size: 28,4 MB → (HD quality)

Animations are on the CD-ROM located on the back cover.

4.2.1 Limitations of the teaching model

The MoTc animation has several limitations:

- **Amounts of columns, ions and molecules:** In the real world, amounts of columns, ions and molecules is considerable higher.

- **Beta radiation:** Beta radiation is visualized using transparent particles. The visualization is the animator's mental model of the phenomena. Also the amount of particles is a vigorous simplification.

- **Calculation level:** Molecules and ions are calculated with Spartan 08 modelling software using semi-empirical calculations. Aluminium oxide columns are taken from free chemical calculations data base (also semi-empirical level).

- **Colours of the atoms:** In a real world, atoms do not have colours. Atom colours in this animation are globally used general atom colours with one exception. Mo and Tc are next to each other and in periodic table and also in global the atom colour system, so in order to see which atoms are molybdenum and which technetium, the green properties of molybdenum are increased (see figures 19 & 20).

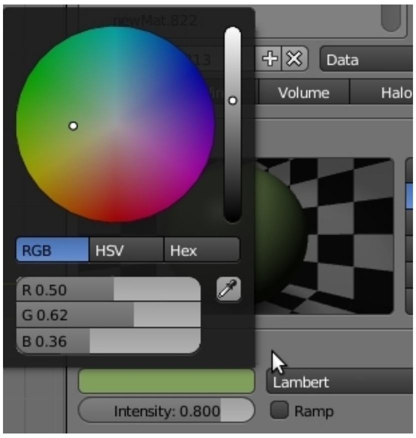


Figure 19. *Mo atom colour*

Figure 20. *Tc atom colour*

- **Movement calculations:** All the movement in the animation is based on the animator's modelling not on calculations.
- **Gamma radiation:** Gamma radiation is visualized as a circular flash. This is also the animator's mental model and a vigorous simplification.
- **Scene:** The scene is a simplified representation of the processes inside the generator.
- **Sizes of the atoms:** Atom sizes in aluminium oxide columns are smaller than other atoms, because the spectator's attention is attempted to draw to molybdenum and technetium ions.
- **Time line:** The time line is also the animator's visualization of the decay process.

4.2.2 Technical details of the final MoTc -animation

Table 3. *Comparison of the technical details between the storyboard and the final version*

Category	Storyboard	Final version	Explanation / reason
Length	**52**	**56**	Legend + end scene
Frames	**1300**	**1400**	Legend + end scene
Scenes	1) Start + overview 0-10 2) Rotation 11-15 3) Zoom in 16-28 4) Zoom out 29-33 5) Elution and ion exchange 34-52	1) Start + overview 0-12 2) Rotation 13-17 3) Zoom in 18-30 4) Zoom out 31-35 5) Elution and ion exchange 36-52 **6) End 53-56**	The end scene was created so that the spectator can visualize the whole picture once more
Frames / second	25	25	-
File format	avi (xvid)	avi (xvid)	-
Beta particles	11 emitter 15-20 particles / emitter life 12 frames	11 emitter 15-20 particles / emitter life 12 frames	-
Gamma rays	**8 flashes** 1000 particles **Life 13 frames**	**6 flashes** 1000 particles **Life 15 frames**	The first gamma flash was removed because of the narration The first elution scene flash was removed in order to emphasize the NaCl flow Life was increased from 13 frames to 15 frames to achieve a longer flash
Background	Black	Black	-

5. Summary and conclusions

The main result of this design research was a high-quality research-based MoTc animation. The first problem analysis revealed that this field only had a few earlier visualizations and some of them were low quality. This animation offers new ways to visualize beta and gamma radiation. Animation was designed after a careful study of earlier research literature and the designing process followed the guidelines of good chemistry animation manufacturing procedures. The animation lasts under 60 seconds, the understanding is supported by a text narration and it is tested by experts [7]. The designing process is also carefully documented and the animation designing has been made in a consensus between the vendor and the customer [1,2,3]. This consensus model is also a teaching model with several possibilities and challenges, which are important when using the animation (see chapter 4.2.1 and [3]).

In the future, the natural way to continue with the project is to carry out a visualization case study. This animation represents a state of the art visualization of this field and will give a new perspective to radiation decay visualizations in a global scale. Therefore it would be interesting to study 1) how this animation effects the understanding of the chemistry inside the MoTc generator and 2) how the possible customers experience the animation.

References

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