

System: Chemistry

Overview / Scope

The Chemistry system allows chemical reactions to occur. These reactions can change the substances within a mixture, change the properties of the mixture and have other effects. This document will focus on the internal chemical reaction system to be implemented, including:

- Definitions relevant to the chemistry system
- The chemistry simulation loop
- System Inputs (Actions)
- System Processes (Chemical reactions)
- System Outputs (Effects)
- Technical notes

It does not cover specific interactions with chemistry paraphernalia, although it does mention some basic interactions as examples. Nor does it cover the job role of the chemist on the station, noting that chemistry can be a core mechanic for several roles (chemist, scientist, bartender, traitor).

Changelog

[illegible]

Definitions

Substance. This refers to a homogeneous chemical composition. This may be an element (e.g. Nitrogen, Oxygen), a compound (e.g. Nitrogen Dioxide, Benzene) or a complex mix of different compounds (Vodka, Blood). Substances are not directly interacted with by players during the game – they are simply a data template. A Substance is specific to its state – for example: Water and Ice are considered different substances.

Substance properties. All Substances have particular properties. Generally these are set values; however, some of these may be dependent on the temperature of the mixture that they are in. Density and solubility can change with temperature. Substance properties include:

- **Name.** The name of the substance.
- **Molar Mass.** The mass of one mole of the substance. (grams / mol)
- **Colour.** The colour of the substance (including transparency).
- **Specific Heat Capacity.** The energy required to raise temperature. (Joules / mol / °C)
- **State.** Solid, Liquid, or Aqueous.
- **Density.** The mass relative to the volume (grams / L; equivalently kg / m³)
- **Solubility in water.** The maximum amount of the substance which can be dissolved in water (for aqueous Substances only).

Substance attributes. Substances can have additional attributes which influence any mixtures that they are in. They are quite similar to traits. Generally, attributes will be coupled with a numeric quantity indicating the relative significance of that attribute.

- Example 1. Vodka has an "Alcoholic" attribute, to quantify the effect on a player when consumed.
- Example 2. Dye has a "Colour Intensity" attribute, so that adding even a small amount of dye to a substance will substantially influence its colour.
- Example 3. Ethanol has a "Flammable" attribute, to indicate its relative susceptibility to being ignited by contact with fire.
- Example 4. Hydrogen sulfide has a "Foul odour" attribute, which can be used to detect its presence by smelling.

Mixture. Simply put, a mixture is a collection of one or more substances. Unlike substances, mixtures can be interacted with directly by the player. A mixture does not inherently know about the substances that make it up, although its own properties and traits are largely derived from them.

Mixture properties. Mixtures have the following properties:

- **Volume.** The total volume of all solid, liquid and aqueous substances within the mixture.
- **Temperature.** How hot the mixture is. This is separate from the temperature of the surrounding atmosphere.
- **Mass.** The mass of the mixture.
- **Heat capacity.** Energy required to heat up the mixture by one degree. Derived from the specific heat capacity of constituent substances.
- **Colour.** The colour of the mixture.

Mixture traits. Mixtures can have a range of traits. These traits can be granted (or removed) as a result of the relative weighting of constituent substances' attributes. The traits can also be added as a result of chemical interactions occurring.

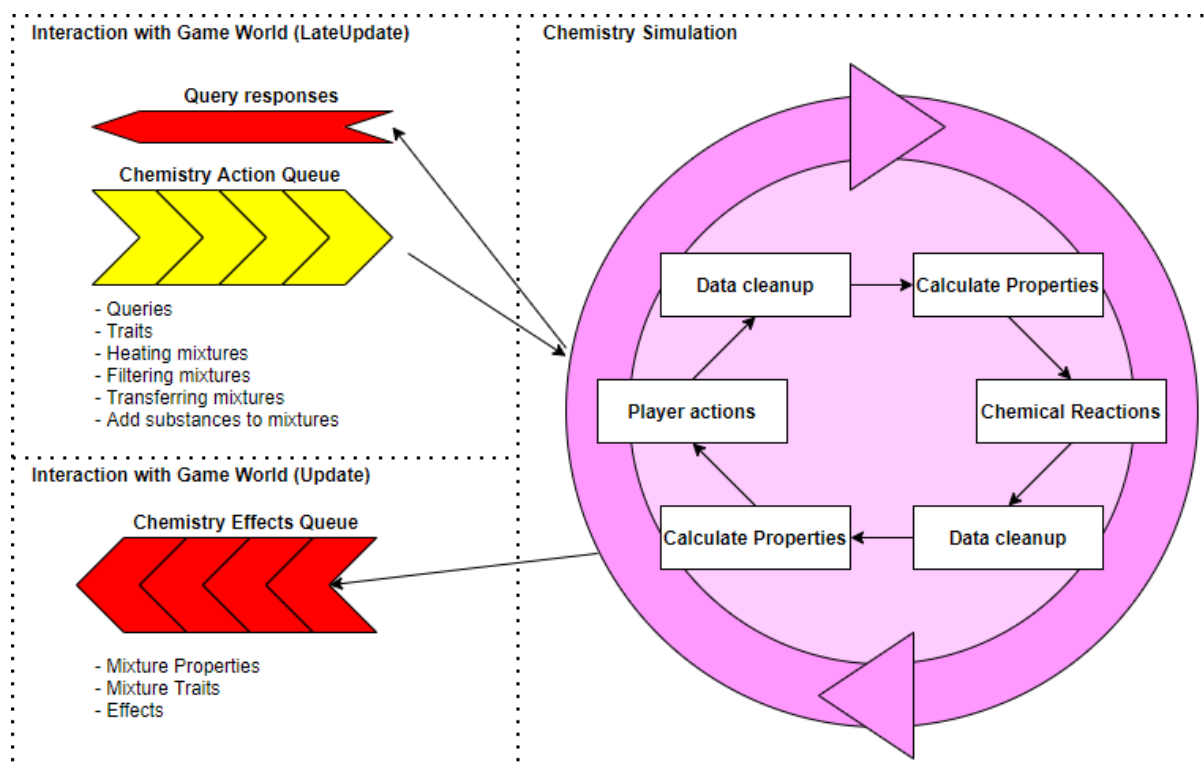
- Example 1. A mixture contains 98% ethanol (which has "Flammable" attribute) and 2% water (which does not). This mixture will have the "Flammable" trait.
- Example 2. A mixture contains 2% ethanol (which has "Flammable" attribute) and 98% water (which does not). This mixture will not have the "Flammable" trait.
- Example 3. A mixture with the "Flammable" trait is exposed to an ignition source. It will then be given the "Burning" trait.

Reaction. These are the heart of the Chemistry system, and govern how reagents will transform. Reactions will be limited by the relative smallest reagent required. Reactions consist of:

- **Reagents.** This is a collection of Substances (and their proportions) which make up a reaction. A reaction requires at least one reagent, and may have several.
- **Products.** These are the Substances (and their proportions) produced by the reaction. A reaction requires at least one product, and may have several.
- **Conditions:** A reaction may (but does not have to) have particular conditions or catalysts which must be met for the reaction to occur. These include minimum / maximum temperatures, minimum / maximum pH, minimum reactant ratio thresholds, being triggered by certain traits (e.g. shaken, stirred, exposed to an ignition source, exposed to environmental oxygen) etc.
- **Energy production.** Reaction may be endothermic, exothermic or neither. The energy gained or lost in the reaction will manifest as heat, which will be determined by the mixture heat capacity.
- **Rate constant.** Some reactions are near-instantaneous, but others take quite a bit of time to complete. Generally, the rate constant and the reactant concentrations will determine the speed of the reaction.
- **Effects.** A specific effect produced whenever this reaction occurs. For example, this could include adding the "Burning" trait to the mixture, or transforming a substance container into a cocktail glass when the cocktail is mixed.

Chemistry simulation loop

The chemistry system is depicted below.



The best way of interpreting this diagram is that everything on the left hand side is how mixtures interact with the game world (players, containers, objects, atmosphere, other mixtures) while the right hand side simulates the chemical processes occurring within individual mixtures only.

It is important to understand that the only way of inputting information into the chemistry simulation is via the chemistry action queue. This queue can be added to at any time, but is only processed during LateUpdate(), so queries will not be able to provide an immediate response.

The chemistry simulation is container agnostic, and will continue to calculate chemical reactions without considering any such restraints. For example, the chemistry simulation may determine the volume of a mixture to be 280mL. If the mixture is in a beaker (container) with only a 250mL capacity, it is the responsibility of the beaker to spill (or delete) the excess 30mL, which it must do by adding a "Transfer Mixture" action to the chemistry action queue. By making the simulation container agnostic, it allows a huge degree of flexibility about what can be used as a container. For example: **bags, food and organs could all be considered to be substance containers if desired.**

System Inputs (Chemistry actions)

The game world can perform a variety of actions to interact with the chemistry system. These actions are:

- **Transferring a mixture to another mixture.** When a mixture is transferred, each of its component Substances are transferred to the new mixture. This can include the complete transfer of the mixture, or just transferring a proportion of its volume. When a mixture is transferred, the temperature of the combined mixture will be the heat capacity weighted average of the two mixtures.
 - Example 1. Adding a 70°C mixture containing 10g of water to a 20°C mixture containing 40g of water will produce a 30°C mixture containing 50g of water.
 - Example 2. Adding a 40°C mixture containing 10g of water (specific heat: 4.186 J / g / °C) to a 0°C mixture containing 10g of ethanol (specific heat: 2.46 J / g / °C) will produce a mixture of approx 25.2°C. Note that the resulting temperature is closer to the original temperature of water because of its higher heat capacity.
- **Adding a substance to a mixture.** This is simply adding an amount of a substance into a mixture. The substance simply becomes the temperature of the mixture it goes into. **Note: This functionality will be deprecated – only mixtures should be able to be added to mixtures.**
 - Example. Adding 10 mol of water to a 20°C mixture containing 40 mol of water will produce a 20°C mixture of 50 mol of water.
- **Heating / cooling a mixture.** This is simply adding or removing heat energy from a mixture. The heat energy added or removed will be indicated in Joules. The actual temperature change of the mixture will be determined by its heat capacity.
 - Example 1. Adding 500 Joules of energy to a 20°C mixture containing 100 g of water (heat capacity of mixture: 418.6 J / °C) will raise its temperature by approx 1.2°C to 21.2°C.
 - Example 2. Removing 500 Joules of energy from a 20°C mixture containing 100 g of ethanol (heat capacity of mixture: 246 J / °C) will lower its temperature by approx 2°C to 18°C.

Developer Guide: Types of heat energy transfer

Energy (Instantaneous). Adds the defined quantity of heat energy (J) to a mixture. The two calculated examples are indicative of this type of transfer. It is mostly used internally by the chemistry simulation. Could also be used for particular situations in-game. Example: A single shot from a laser weapon hitting a mixture would apply a

set amount of energy to the mixture.
Energy Per Second. Adds the defined quantity of heat energy per second (J / s). This makes the simulation independent of the time between chemistry simulation steps. Example: A continuous beam from a laser weapon hitting a mixture would apply a set amount of energy per second to that mixture.
Energy Per Second (SA:V proxy). Adds the defined quantity of heat energy to each litre of substance each second ($\text{J} / \text{L} / \text{s}$), scaled by a proxy for the surface area to volume ratio. Useful for situations where you might have mixtures of vastly different volumes, but you want a somewhat consistent heating effect. Example: Mixtures in a coolroom may have their heat energy reduced in this way, to prevent major changes to the cooling rate between a 50L tub filled with one mixture, and a 250mL beaker filled with another. The SA:V proxy ensures that the beaker will cool more quickly than the tub, but not unrealistically so.
Temperature (Instantaneous). Adds the defined temperature to the existing temperature ($^{\circ}\text{C}$). Generally not recommended.
Temperature Per Second. Adds the defined temperature to the existing temperature, independent of time ($^{\circ}\text{C}/\text{s}$). Generally not recommended.
Set Temperature. The mixture will be set at the defined temperature ($^{\circ}\text{C}$), irrespective of the existing temperature. This should generally not be used in gameplay, but may be used by the chemistry system itself. Example: Setting the initial temperature of all mixtures in the station at round start.

The preferred heat energy transfer methods are the energy-based (rather than temperature-based) methods and the time-independent methods (i.e. "Per Second" rather than instantaneous). The temperature-based methods completely disregard the chemical properties (i.e. heat capacity) of a mixture in their calculations. The instantaneous methods are subject to inconsistent results if applied incorrectly. For example, a blowtorch applying energy to a mixture via an instantaneous method will find that the temperature change of that mixture will be directly proportional to frame rate.

- **Adding a trait trigger to a mixture.** Traits can be applied to mixtures each frame to trigger reactions to occur. These traits will not be maintained by the system (i.e. they will need to be re-sent every frame that they are required). Generally, traits will be added via the interaction system or via physics triggers in-game.
 - Example 1. Interacting with a mixture (as the Interaction Target) containing kahlua and vodka while holding a spoon (as the Interaction Source) will cause you to stir the mixture, and send a "Stirred" trait to the mixture. If the kahlua and vodka are present in the correct ratios, they

will react to form a Black Russian cocktail. Once the player ceases the stirring interaction, the mixture will no longer have the "Stirred" trait.

- o Example 2. If the flame of a blowtorch intersects the mesh of a mixture instance, a "Ignition Source" trait will be sent to the mixture. If that mixture is flammable, it will cause other chemical reactions to occur. Although the mixture does not maintain the original "Ignition Source" trait once the blowtorch is removed, it will get the "Burning" trait while the reactions are occurring, and will be an ignition source in its own right.
- **Filtering a mixture.** Mixtures can have all components of a particular state filtered away to another mixture.
 - o Example. A beaker (Interaction Source) containing a mixture can be poured through a fine sieve (Interaction Target) into a second beaker. After this interaction, the sieve would have a mixture containing all solid substances from the original mixture, and the second beaker would contain all the liquid and aqueous substances from the original.
- **Queries.** Players have only a very limited knowledge of a mixture by default, such as its volume and colour. For a player to get more detailed information, they need to query the chemistry system.
 - o Example. A chemist wearing spectroscopic scanner goggles is able to query the chemistry system to identify the exact composition of substances within a mixture.

The order that the player actions are dealt with by the substance system is queries, traits, heating/cooling mixtures, filtering mixtures, transferring mixtures and adding substances to mixtures.

System Processes (Chemical reactions)

To be inserted.

System Outputs (Chemistry effects)

To be inserted.

Technical notes & implementation details

The chemistry simulation loop is run as a data driven simulation using the Unity Jobs System and Burst compiler. Detail to be inserted.