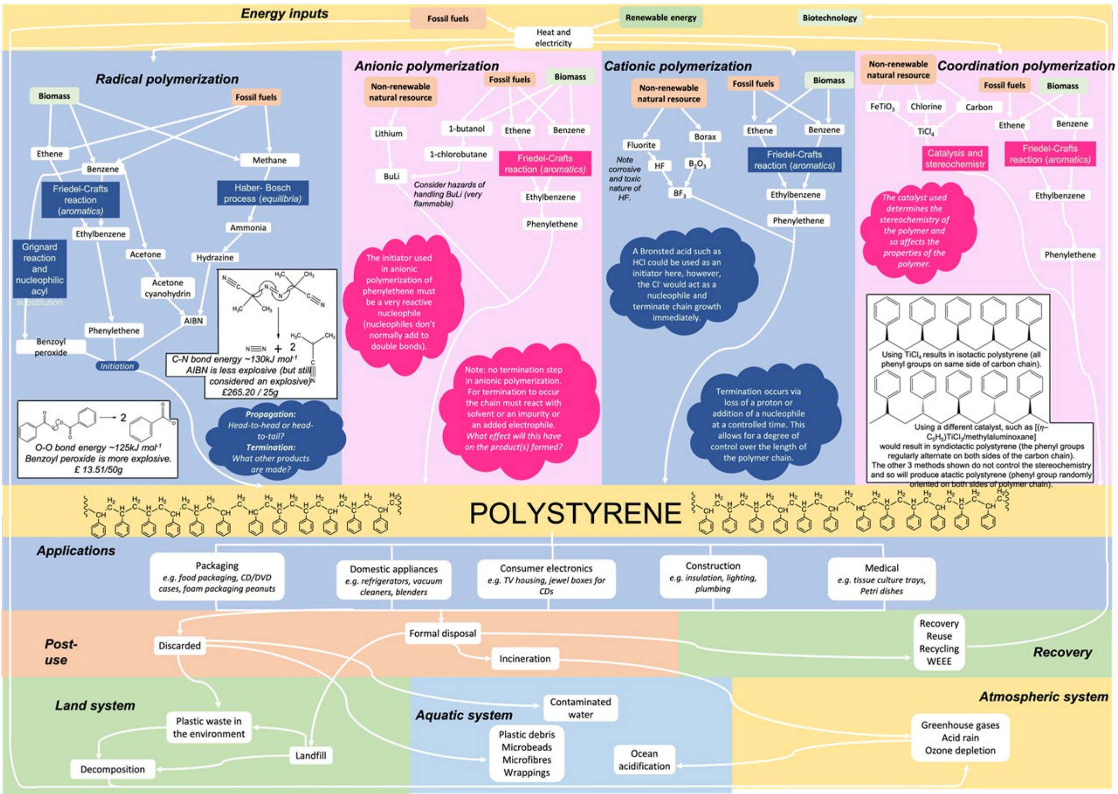
Electronic Supplementary Material (ESI) for Chemistry Education Research and Practice.

SOCME shown



Transcript

1. One very useful tool for visualising a system is a systems-oriented concept map extension or SOCME. Here, we will see a SOCME for the synthesis of polystyrene.

2. Within this SOCME, we will consider the different methods for this synthesis: radical, anionic, cationic and coordination polymerisation techniques will all be displayed as separate subsystems.

3. First, we will examine the synthesis via radical polymerisation. This subsystem displays the routes to phenylethene and two possible initiators from either fossil fuels or biomass. The synthesis of ethylbenzene from ethene and benzene involves a Friedel-Crafts alkylation step, which could be used to introduce students to ideas of aromaticity and reactions of aromatic molecules.
The synthesis of ammonia (which is a precursor for the synthesis of AIBN) could introduce the Haber-Bosch process and so ideas of equilibria, and the synthesis of benzoyl peroxide involves a Grignard reaction and nucleophilic acyl substitution, therefore these syntheses involve methods suitable for linking a number of different areas of the undergraduate chemistry curriculum.
Furthermore, when considering which initiator to use, ideas of bond strength, cost and safety can also be investigated.
So far, we have only discussed the initiation step of this polymerisation technique. Propagation and termination steps allow for consideration of selectivity and uses of any unwanted by-products.

4. Here, we see the subsystem depicting the anionic polymerisation route to polystyrene. Again, the routes to phenylethene and an initiator are displayed.
In this method, the initiator used must be a very active nucleophile as nucleophiles don't normally add to double bonds. BuLi is used here, however the hazards of BuLi should be considered as it is very flammable.

There is no official termination step in anionic polymerisation. For termination to occur, the chain must react with solvent, an impurity or an added electrophile. Students could be encouraged to consider the possible effects on reaction metrics as a result of this.

5. Now, we will examine the cationic polymerisation subsystem. In this example, BF_3 is used as the initiator for the polymerisation, and the corrosive and toxic nature of this chemical should be noted. BF_3 is a Lewis acid; a Brönsted acid such as HCl could be used as an initiator here but the Cl^- ion would act as a nucleophile and terminate chain growth immediately.
   In the example shown, termination would occur via loss of a proton or addition of a nucleophile at a controlled time. This allows for a degree of control over the length of the polymer chain.

6. Finally, we will consider polystyrene synthesis via coordination polymerisation. In the example shown, a $TiCl_4$ catalyst is used in place of an initiator. However, other catalysts may also be appropriate. The choice of catalyst determines the stereochemistry of the product and so this polymerisation method can introduce students to both catalysis and ideas of stereochemistry. The other 3 polymerisation methods do not determine the stereochemistry of the product.

7. All of these methods require heat and electricity. This can be obtained from fossil fuels or renewable energy.

8. Now that we have considered its synthesis, we can move onto applications of polystyrene. Examples include packaging, domestic appliances, consumer electronics, construction and medical applications.

9. Once used, the polystyrene must be disposed of. It may be discarded or disposed of formally via incineration. The disposal method used will determine any environmental effects.

10. First, we will consider the effects to land and aquatic systems. If the polystyrene is just discarded, this would lead to plastic waste in the environment and contaminated water potentially containing plastic debris, microbeads, microfibres and/or wrappings.
    If the polystyrene was put in landfill, it may decompose or it may just remain there as plastic waste.

11. If the polystyrene was to be incinerated, this could lead to the generation of greenhouse gases, acid rain, ozone depletion and ocean acidification.

12. As shown on the SOCME, the atmospheric system is also affected by other subsystems. Decomposition, heat and electricity and the use of fossil fuels also contribute to these effects.

13. However, the polystyrene may also be disposed of using the methods shown here in the recovery subsystem.
    Recovery, reuse and recycling may reduce the environmental impacts on the system. Also, if waste electronic and electrical equipment (WEEE) is recovered and recycled to obtain critical elements used in catalysis for example, this would also aid in reducing negative environmental impacts of this system.

14. As you can see, this SOCME shows how the synthesis of polystyrene can be considered as a system with relationships between each of the subsystems and can be used to help introduce students to think about systems more holistically.