

MIT WORLD PEACE UNIVERSITY

Principles of Green Technology  
Fourth Year B. Tech, Semester 1

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PRINCIPLES OF GREEN TECHNOLOGY

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ASSIGNMENT 3

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November 8, 2024

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## 1 Microwave-Assisted Reactions

Microwave-assisted reactions utilize microwave radiation as a heating source to accelerate chemical reactions. This method has gained popularity due to its efficiency and selectivity. Here are some key points:

- **Energy Transfer:** Microwaves directly interact with polar molecules in the reaction mixture, generating heat through dipole rotation and ionic conduction. The energy transfer can be described by the equation

$$P = \epsilon'' E^2 f$$

where  $P$  is the power absorbed,  $\epsilon''$  is the dielectric loss factor,  $E$  is the electric field strength, and  $f$  is the frequency of the microwave.

- **Rapid Heating:** Microwave heating allows for uniform, rapid heating which reduces reaction time significantly compared to conventional heating. This rapid heating can be modeled by the Arrhenius equation

$$k = A e^{-\frac{E_a}{RT}}$$

where  $k$  is the rate constant,  $A$  is the pre-exponential factor,  $E_a$  is the activation energy,  $R$  is the gas constant, and  $T$  is the temperature.

- **Selective Heating:** Microwaves selectively heat specific reactants or solvents, enabling targeted reactions and reducing side reactions. This selectivity can be advantageous in multi-component systems where only certain components absorb microwave energy.
- **Enhanced Reaction Rates:** Increased molecular motion at high temperatures enhances reaction rates, often yielding higher product selectivity and purity. The increased reaction rates can be quantified by the collision theory, which states that the rate of reaction is proportional to the number of effective collisions per unit time.
- **Environmental Benefits:** Microwave-assisted reactions are often more energy-efficient, reducing the need for harsh chemicals or excess solvents. This aligns with the principles of green chemistry, which aim to minimize the environmental impact of chemical processes.

## 2 Photochemical Reactions

Photochemical reactions are chemical reactions initiated by the absorption of light. They play a critical role in organic synthesis, environmental chemistry, and biological processes. Important points include:

- **Energy Source:** Light (UV or visible) is used as an energy source to excite reactant molecules, leading to reactions that may not occur under thermal conditions. The energy of a photon is given by

$$E = h\nu$$

where  $h$  is Planck's constant and  $\nu$  is the frequency of the light.

- **Reaction Mechanism:** Absorption of photons causes electronic excitation, often resulting in bond dissociation or electron transfer. The Jablonski diagram is commonly used to illustrate the electronic states of a molecule and the transitions between them.

- **Selectivity Control:** Specific wavelengths of light can target particular bonds or functional groups, allowing for high reaction selectivity. This selectivity can be exploited in synthetic chemistry to achieve desired products with minimal side reactions.
- **Applications in Synthesis:** Common in the synthesis of complex molecules, particularly in creating cyclic structures and rearrangements. Photochemical reactions are used in the synthesis of vitamin D, fragrances, and pharmaceuticals.
- **Green Chemistry Aspect:** As it often requires less energy and reduces waste, photochemistry aligns well with sustainable chemistry principles. The use of sunlight as a renewable energy source further enhances the sustainability of photochemical processes.

### 3 Inherently Safer Design

Inherently safer design (ISD) is a methodology in process engineering aimed at minimizing hazards by designing processes and equipment that are fundamentally less likely to cause accidents. Key principles include:

- **Minimization:** Reduce the quantity of hazardous substances involved in the process. This can be achieved by using smaller reactors or continuous processing techniques.
- **Substitution:** Replace hazardous substances or processes with safer alternatives, such as using less toxic materials. For example, using water as a solvent instead of organic solvents.
- **Moderation:** Use less hazardous conditions, such as lower temperatures and pressures, to minimize risk. This can be quantified by the equation

$$P = \frac{nRT}{V}$$

where  $P$  is the pressure,  $n$  is the number of moles,  $R$  is the gas constant,  $T$  is the temperature, and  $V$  is the volume.

- **Simplification:** Design systems to be less complex, thereby reducing potential failure points. Simplified systems are easier to operate and maintain, reducing the likelihood of human error.
- **Methodology:** ISD methodologies involve hazard identification, risk assessment, and process optimization to design safety into the process. Techniques such as HAZOP (Hazard and Operability Study) and FMEA (Failure Modes and Effects Analysis) are commonly used.

### 4 Supercritical Carbon Dioxide as a Solvent and Decaffeination Process

Supercritical carbon dioxide ( $scCO_2$ ) is a popular solvent due to its unique properties near the critical point (31.1°C, 73.8 bar). It is particularly useful in extraction processes, such as decaffeination. Key aspects include:

- **Solvent Properties:** Supercritical  $CO_2$  has both gas-like diffusivity and liquid-like solvating power, making it an effective solvent for nonpolar and moderately polar compounds. The solubility of compounds in  $scCO_2$  can be described by the equation

$$\ln S = A + \frac{B}{T}$$

where  $S$  is the solubility,  $A$  and  $B$  are constants, and  $T$  is the temperature.

- **Environmental Benefits:** CO<sub>2</sub> is non-toxic, non-flammable, and recyclable, making it a sustainable alternative to organic solvents. The use of scCO<sub>2</sub> reduces the environmental impact of chemical processes by minimizing solvent waste.
- **Decaffeination Process:** Coffee beans are exposed to scCO<sub>2</sub>, which selectively dissolves caffeine while leaving most flavor compounds intact. The process involves circulating scCO<sub>2</sub> through the beans at high pressure, followed by depressurization to separate the caffeine.
- **Efficient Extraction:** The process is both fast and effective, achieving high yields without the need for harsh chemicals. The efficiency of extraction can be enhanced by optimizing parameters such as temperature, pressure, and flow rate.
- **Applications Beyond Decaffeination:** scCO<sub>2</sub> is widely used in essential oil extraction, pharmaceutical purification, and food processing. Its versatility and environmental benefits make it a valuable tool in various industries.

## 5 Process Intensification

Process intensification aims to make chemical processes more efficient, compact, and sustainable by fundamentally improving the equipment and methodologies used. Essential points include:

- **Enhanced Efficiency:** Process intensification seeks to increase energy and resource efficiency, often reducing operating costs. This can be achieved by improving heat and mass transfer rates, reducing reaction times, and minimizing energy consumption.
- **Equipment Minimization:** Combining multiple process steps into a single apparatus or integrating functions to reduce equipment size. Examples include microreactors, which offer high surface area-to-volume ratios, and multifunctional reactors that combine reaction and separation processes.
- **Improved Safety:** Smaller equipment and intensified processes can reduce hazardous inventories, leading to safer operations. The reduced scale of equipment also minimizes the potential impact of accidents.
- **Sustainability Benefits:** By reducing energy, waste, and raw material usage, process intensification aligns with environmental and economic goals. The use of renewable energy sources and waste valorization further enhances sustainability.
- **Application Areas:** Includes technologies like microreactors, heat exchangers, membrane reactors, and hybrid separation techniques. These technologies offer improved performance and flexibility compared to traditional equipment.

## 6 In-Process Monitoring and Analysis

In-process monitoring and analysis involves the continuous assessment of reaction parameters during production to ensure product quality and optimize efficiency. Notable points include:

- **Real-Time Data:** Provides real-time data on reaction parameters such as temperature, pH, pressure, and concentration. This data can be used to make immediate adjustments to the process, ensuring optimal conditions are maintained.
- **Quality Control:** Ensures that each stage of production meets quality standards, allowing for immediate adjustments. This reduces the likelihood of producing off-spec products and minimizes waste.
- **Improved Efficiency:** Helps in optimizing processes by monitoring reaction kinetics, thus reducing waste and improving yield. The use of advanced analytical tools allows for precise control of reaction conditions.
- **Analytical Tools:** Common methods include spectroscopy, chromatography, and mass spectrometry for in-line and on-line monitoring. These techniques provide detailed information on the composition and properties of reaction mixtures.
- **Automation and Control:** In-process monitoring can be integrated into automated control systems for more precise and consistent process management. This integration enhances process reliability and reduces the need for manual intervention.