Scale-Up of Chemical Engineering Process

Chapter 6: Simulator

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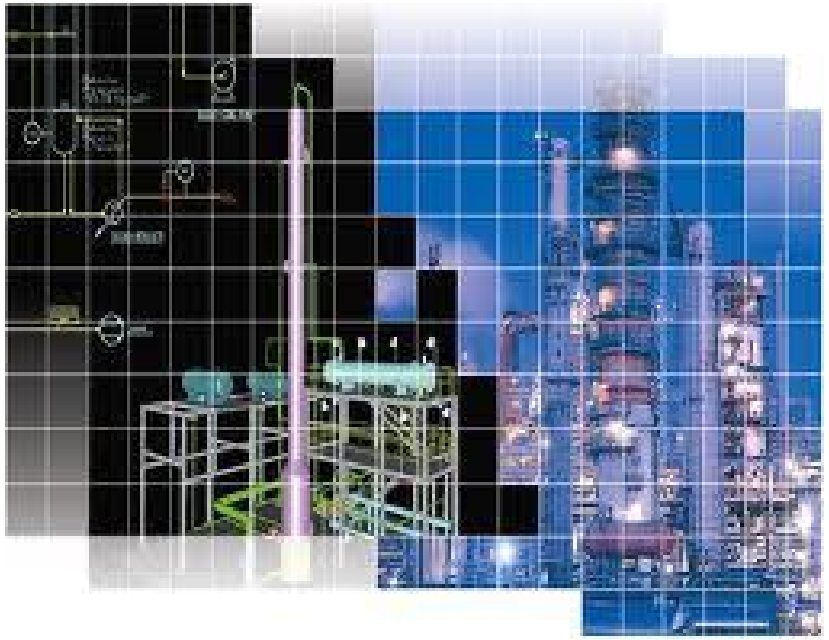
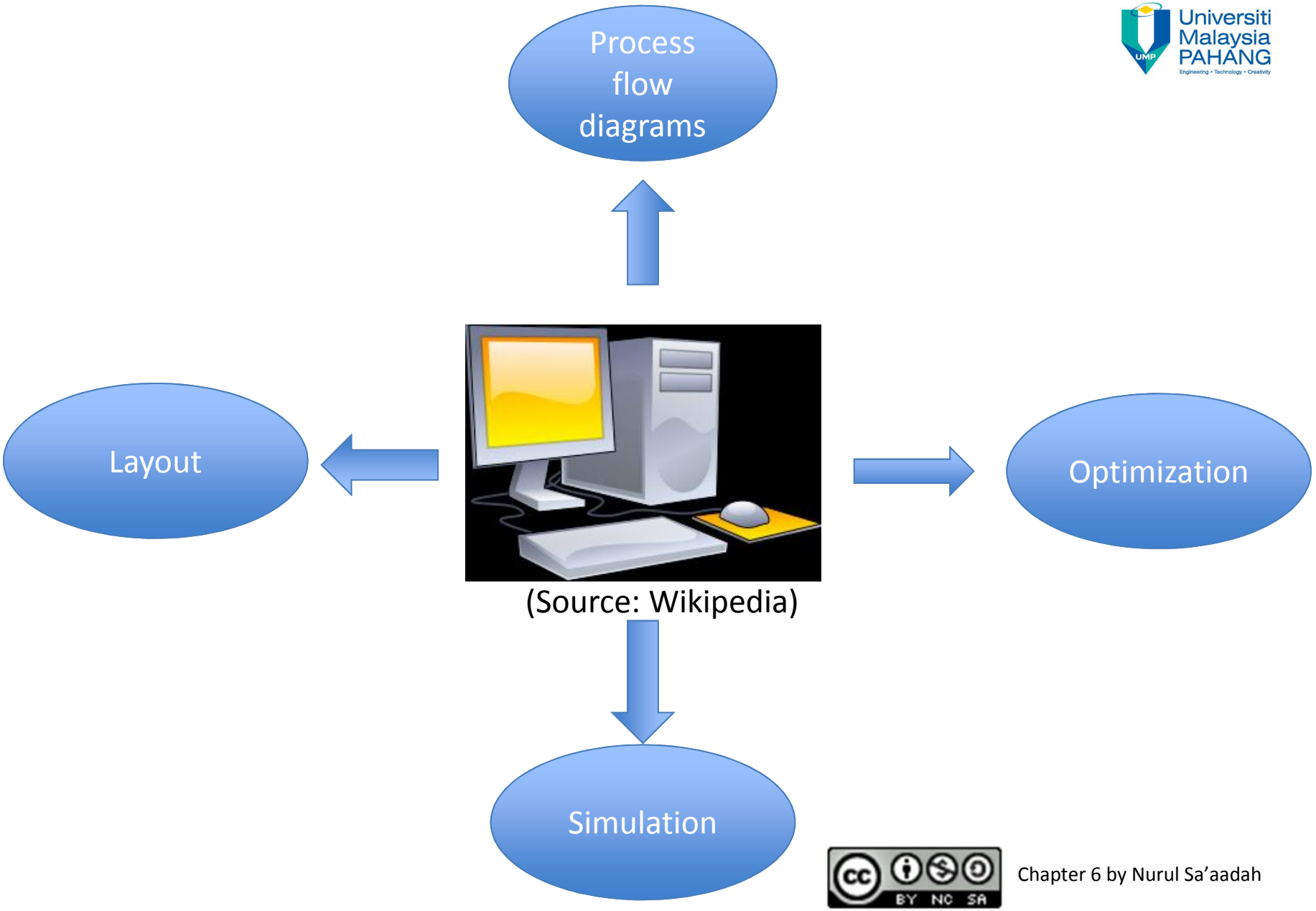
General Information

- **Process simulator is a very useful tool in plant design & scale-up;**
- **Helps reduce time & cost;**
- **Difference between steady state and dynamic simulation;**
- **Simulator based on assumptions;**
- **Human error leads to simulation errors**

COMMERCIAL PROCESS & PLANT SIMULATOR

- ASPEN PLUS
- HYSIM (HYSIS)
- CHEMCAD
- PRO/II
- SUPERPRO
- PROSIM





(Source: Wikipedia)

Chemical Property Estimation

- **KEY REQUIREMENT – accurate in representing properties of the chemical species.**
- **KINETIC DATA – rate equations, activation energy**
- **THERMODYNAMIC PROPERTIES – enthalpy, entropy, fugacity etc.**
- **TRANSPORT PROPERTIES – diffusion coefficient, thermal conductivities, viscosities etc.**

Tips for Simulation

- **Treat the simulation as experimental setup;**
- **Choose the right thermo model;**
- **First, input only the required data to do m.e.b.;**
- **Do not violate mass balance (eg. distillation specification);**
- **Make sure the simulation converge;**
- **Reason not converge – incorrect equipment specification or inappropriate thermo model**

Author Information

Credit to the author:

Prof Ir Dr Badhrulhisham Abdul Aziz

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