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ASPEN Plus – Introduction. Part 1: properties of pure substances

Start with general simulation and add these data (Bookmark "Properties"):

Components: water, ethanol, propan-2-ol, benzene, toluene, cyclohexanone, cyclohexanol

Models ("Methods") describing properties of pure substances: IDEAL, WILSON, NRTL

Properties of pure substances.

1. Examine the dependence of molar evaporation enthalpy of water and ethanol in the temperature range 80 – 260 °C. Discuss the curve shape and why it becomes constant.
2. Create a diagram of the dynamic viscosity of liquid and gaseous benzene for the temperature range 35 – 60 °C. Discuss the dependence of viscosity of both phases on temperature.
3. Determine if toluene can form explosive mixture with air at 32 ° C (see the MSDS for the explosion limits of toluene).
4. Find the boiling point of propan-2-ol at 5 atm.

BONUS: Equilibria (l) – (g) of binary mixtures

1. Create a *T-x-y* diagram for the ethanol-water system.

Save your project on HDD, we will continue with this simulation at Seminar 2.

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ASPEN Plus – Introduction. Part 2: properties of Binary mixtures

Continue with simulation from Seminar 1 (Load it to Aspen Plus simulation).

Equilibria (l) – (g) of binary mixtures

1. Create a *T-x-y* and *y-x* diagrams for the propan-2-ol – water system
    a. Assuming the ideal behaviour of both phases
    b. Assuming that the behaviour of liquid mixtures is described by NRTL model.

    What is the composition of the azeotropic mixture in gaseous phase at the boiling temperature?

2. Construct a *y-x* diagram for the liquid – gas equilibrium of cyclohexanone-cyclohexanol mixture for the pressures: 1, 0.5 and 0.1 atm. What pressures will you use for the separation of both components by distillation?

Adiabatic evaporation

Solution of 10 % ethanol (mass) in water is fed at a rate of 2 t / h at a pressure of 0.5 MPa and the boiling temperature to a single-stage “instantaneous distillation”; apparatus is operating at atmospheric pressure.

- Calculate the weight percentage of the vapours leaving the system, while it operates adiabatically.
- What heat output would be needed to evaporate half of the mixture?

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ASPEN Plus – Distillation. Part 1: Sensitivity analysis.

Vacuum fractional distillation

In the process of oxidation of cyclohexane is produced a mixture, containing cyclohexanol and cyclohexanone in the molar ratio of 2:1. Cyclohexanone is then purified to 85 % (wt.), and the rest of the cyclohexanol is recycled in the process.

1. Design a vacuum rectification column for the mixture. Suppose the packed column has a pressure drop of 1 kPa on the theoretical floor. The deepest acceptable vacuum is 4 kPa for economic reasons.
    a. Assuming that the behaviour of the mixture is described as non-ideal.
    b. Model the column for at least 3 different values of the pressure.

Sensitivity analysis

It is necessary to process 1000 kg per hour of benzene (65% wt.) and toluene mixture. An existing atmospheric rectification column (20 TP) is available. The spraying can be fed to all floors between 8 and 15. A distillate of 98 % wt. purity is required so as a yield of benzene in the distillate of at least 96%.

1. Make a simulation of supposed column
2. Using the Sensitivity Analysis tool, check the effect:
    a. Reflux ratio
    b. Feed stage
    c. Distillate rate
    d. Combinations of these parameters.
3. Using the information obtained under 2), optimize the rectification line.
4. Find the required power of the boiler.

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ASPEN Plus – Distillation. Part 2: optimization

Optimization of fractional distillation

The esterification of acrylic acid with methanol is carried out in an excess of alcohol. The remaining alcohol is extracted from the reaction mixture into water. The 5 t / h extract contains 15 wt. % of methanol is separated from the mixture and returned to the esterification process. Design a device for atmospheric rectification of methanol with the following requirements:

a. Purity of the distillate has to be at least 98 % wt.
b. The distillation residue (waste water) can contain 200 ppm of methanol at maximum

Optimize the column and make an analysis of the process parameters.

1. Find optimal height (by TP) of the column and feed stage.
2. Calculate optimal reflux ratio and the distillate rate.
3. Find the required power of the boiler.
4. Suggest a way of using the heat of the leaving distillation residue.

ASPEN Plus – Chemical reactors. Part 1: chemical equilibrium

Reactor RGibbs

During steam reforming of natural gas, 25 tons of methane per hour and water vapour enter into the reactor, both streams being preheated to 300 ° C, under pressure 2.5 MPa. Use the Benedict-Webb-Rubin state equation (or its derivative) to describe the behaviour of the gases. The chemical reactions in the reactor are:

$$CH_4 + H_2O = 3H_2 + CO$$

$$CO + H_2O = H_2 + CO_2$$

1. Examine the dependency of conversion of methane on the outlet temperature and pressure (recommended limits 500-1000 ° C, 1-3 MPa). Select the pressure to satisfy the process requirement for minimum reactor pressure 2 MPa.
2. For the selected pressure, verify the influence of the temperature and the ratio of ZP / H_2O in the feed on the resulting molar ratio of H_2 to CO in equilibrium mixture (calculated without water).

Reactor REquil

Simulate the adiabatic esterification of acetic acid with methanol in the liquid phase. Select the appropriate model to describe the liquid phase behaviour. The reactor feed is an equimolar mixture of acid and alcohol at an aggregate molar flow rate of 2 kmol / h at 10 ° C.

$$CH_3COOH + CH_3OH = CH_3COOCH_3 + H_2O$$

Optimize the column and make an analysis the process parameters.

1. Find optimal height (by TP) of the column and feed stage.

2. Calculate optimal reflux ratio and the distillate rate.

3. Find the required power of the boiler.

4. Suggest a way of using the heat of the leaving distillation residue.

ASPEN Plus – Chemical reactors. Part 2: kinetics

Tubular Reactor

Simulate the adiabatic esterification of acetic acid with methanol in the liquid phase with the usage of kinetic model. Select the appropriate model to describe the liquid phase behaviour. Consider the reactor as a piston flow tubular reactor that operates in adiabatic mode (the tube is straight with a constant diameter of 50 cm and a length of 10 m). The reactor is fed with an equimolar mixture of acid and alcohol at an aggregate molar flow rate of 2 kmol / h at 10 ° C. From a comparison of the conversion of the starting materials, see if at least 90% of the equilibrium is reached in the reactor. Use experimental approach to simulate the identified kinetic parameters of esterification. Assume that the reactions are always first-order to both of their reactants.

$$CH_3COOH + CH_3OH = CH_3COOCH_3 + H_2O$$

Table 1 Kinetic parameters of esterification of acetic acid with methanol

Reaction	parameter k_0, $dm^3 \cdot mol^{-1} \cdot s^{-1}$	E_A, $J \cdot mol^{-1}$
Forward	$5.00 \cdot 10^{-5}$	500
Back	$1.52 \cdot 10^{-6}$	450

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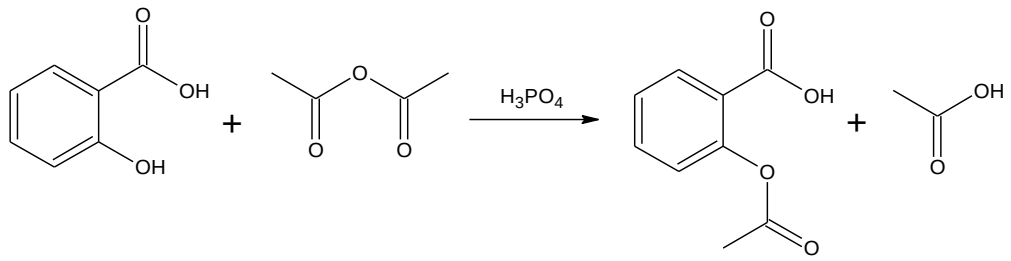
ASPEN Batch Process Developer Part 1 + 2

Transfer of Aspirin manufacture from the laboratory to pilot plant

In the R & D department, you have developed the following procedure for preparing Aspirin:

Compounds	**Equipment**
Acetic acid	Erlenmeyer flask 250 ml
Acetic anhydride	Filter flask 250 ml
Acetylsalicylic acid	Evaporating dish
Phosphoric acid (85%)	
Salicylic acid	
Water	

Reaction :



Workflow:

1. Charge a 250 ml Erlenmeyer flask with:
   3 g of salicylic acid
   6 ml of acetic anhydride
   1 ml of 85% phosphoric acid
   100% salicylic acid is dissolved. The reaction runs with 100% conversion. Final temperature 75 ° C.
2. Add 20 ml of water.
   100% acetylsalicylic acid crystallizes after cooling the flask to 25 ° C
3. The reaction mixture is filtered through a 250 ml filter flask. The crystals are washed with 2.5 ml of water.
4. The crystals are dried on an evaporating dish for 30 minutes at 100 ° C.

Use the Aspen Batch Process Developer simulation program to check the material balance, stoichiometry and yield of the reaction, and convert your progress to a pilot scale.

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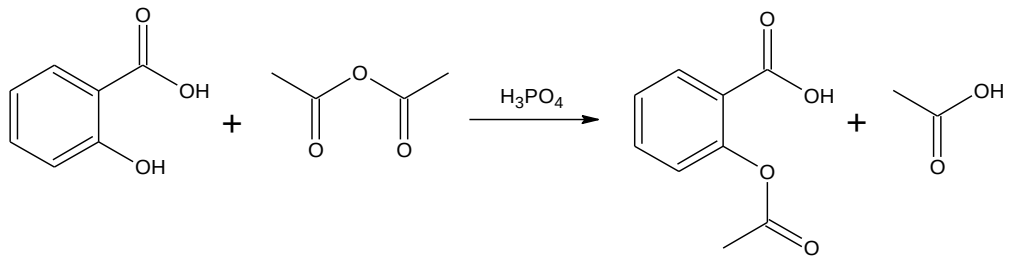

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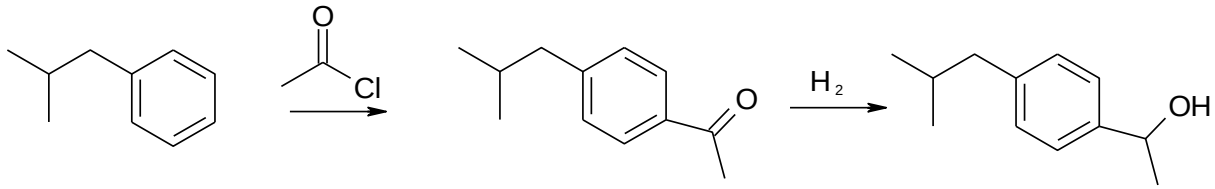
ASPEN Batch Process Developer Part 3 + 4

Production of Ibuprofen

In the R & D department, you have developed the following procedure for preparing Ibuprofen:

Compounds	**Equipment**
Isobutyl benzene	Reactor 100 l
Acetyl chloride	Autoclave 10 l
Hydrogen	4x Tank 500 l

Reaction :



(Create 2 reaction schemes with by-products. Add these compounds into your project. If they aren't in the database, import them via ISIS Draw. Conversion of acylation is 90%)

Workflow:

1. There is one large reactor (100 l) and one smaller autoclave suitable for hydrogenation reactions (10 l) in the operating hall. There are also 4 tanks (500 l). Create your own "facility" and add these devices there.

2. Charge to a larger reactor:
   50 kg of isobutyl benzene
   acetyl chloride in a molar ratio of 1: 1 to isobutyl benzene
   1 kg of AlCl3 catalyst
   The mixture reacts for a total of 3 hours.

3. Distil the resulting reaction mixture directly from the reactor. The volatile components are directed to the first container (100% acetyl chloride, HCl, isobutyl benzene). The resulting "phenone" and other unspecified substances remain in the reactor.

4. Part of the content of second tank transfer to the autoclave (autoclave to fill 8kg of the mixture).
   The mixture is allowed to react (reaction scheme of hydrogenation). Hydrogen is

continuously added in a molar ratio of 1: 1 to a "phenone" which is 100% dissolved in the liquid phase.

5. Resulting reaction mixture is transferred to the third tank.

6. Schedule campaign production with two cycles of acylation reaction and an adequate number of hydrogenations. (Plan Explorer tab)

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ASPEN Batch Process Developer Part 3 + 4

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Compounds	**Equipment**
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Hydrogen	4x Tank 500 l

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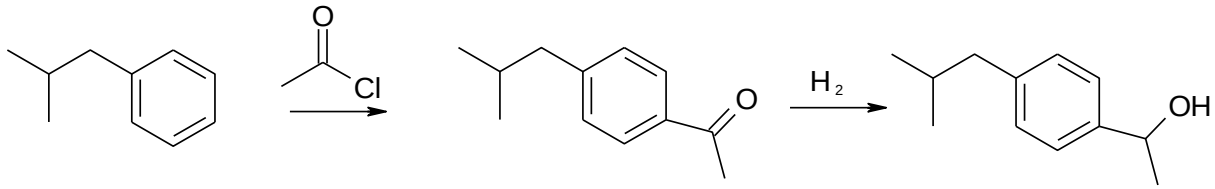

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6. Schedule campaign production with two cycles of acylation reaction and an adequate number of hydrogenations. (Plan Explorer tab)

During weeks 11 to 14 students are working on their projects in small groups (usually 2 to 3 students together). Below are examples of project tasks.

ASPEN Plus – Project

In the pharmaceutical industry, until recently, the production of API did not address the issue of recycling of solvents since the high price of API market was able to cover this aspect. In recent years, with increased competition and the prices of solvents and their subsequent destruction, this issue is becoming topical.

Task

In the production of analgesics, the last part of the synthesis is carried out in toluene. From the viewpoint of the reaction it is required to use toluene with water content below 500 ppm as well as the presence of substances with an OH group normalized below 1 ppm. After the synthesis, the toluene-soluble product is precipitated at 25°C with methanol and then filtered. The factory thus produced 2000 tons/year (working time 8000 h) of toluene-methanol mixture with the concentration of methanol 55 %. These days, the mixture is not separated and is sent to an external company to burn, while the price for this operation is 8500 CZK/ton. The purchase price for methanol is 7000 CZK/ton and for toluene 21 000 CZK/ton. The price of the vapour 6 bar in the factory is 550 CZK/ton. Suggest the process of isolation and compare operating costs with the current state. Due to the properties of the mixture which forms an azeotrope at atmospheric pressure with a minimum boiling point of a 27 % toluene, the mixture cannot be divided by rectification. On the other hand, it is possible to extract the polar methanol from toluene by water and then to distil these separate mixtures. In solving the problem consider the extractor with 5 theoretical plates. The currents resulting from the extraction process by rectification so that toluene contains less than 1 ppm of methanol and 500 ppm of water and methanol contains maximum of 0.5% toluene and 1% water. In the production, there are two atmospheric rectification columns C01 (10 TP) and C02 (20 TP), both with the oriented filling and the spraying conducted in the middle. Expect 20% of heat loss to the surroundings.

ASPEN Batch Process Developer – Project: Production of Ephedrine

Ephedrine (2-(methylamino)-1-phenylpropan-1-ol) is produced by the catalytic reductive amination of phenylacetylcarbinol (1-hydroxy-1-phenyl-propan-2-one) with methylamine (MMA). The reaction is carried out at 100°C for 5 h in toluene in the presence of Pt catalyst at elevated hydrogen pressure. A slight surplus of MMA ensures total conversion of phenylacetylcarbinol. The input toluene solution has a concentration of 120 g / L of phenylacetylcarbinol. After the reaction and the separation of the catalyst, ephedrine is isolated using 36% HCl as the hydrochloride.

Design production of ephedrine under the following conditions in Aspen Batch Process Developer:

- There is an autoclave available with a volume of 400 L (D400).
- The catalyst used is 5% Pt on C in an amount of 1 g per 60 g of substrate.
- There is 30% aqueous solution MMA available.
- Reaction heat of hydrogenation is 100 kJ / mol.
- There is only one filter (bag filter 100) for filtration (catalyst and the product).
- Precipitation is carried out by 36% HCl in a vessel with a volume of 1000 L (V201).
- Heat of hydrochloride formation is 40 kJ / mol.
- Drying of the final product to a moisture content of 1% is carried out at 50 ° C for 5 h.`

Try to simulate other variations of the process. Think of the optimal utilization of the vessels (V201 is too large, wouldn't be possible to make two batches of hydrogenation at once?) and try to simulate the campaign.