

DuDES Checklist

Introduction

This document is a checklist that can be used to consider what each task in a conceptual process requires the equipment to deliver. This can be used as part of the DuDES process. Note that few, if any, tasks will require every entry on this checklist to be specified. There also might be important aspects that are not covered in this checklist: every process has its own individual requirements.

The first consideration for each of the points below should be: "is this relevant to the process task I am considering?" If the answer is "yes", then the question should be answered to the best level of information you have. In many cases order of magnitude answers will be sufficient, particularly for DuDES-Lite. This list of questions will also identify where there are gaps in your knowledge.

Task purpose

- What is the purpose of the task?

Material balance & residence time

- Mass flow or mass per batch of each material fed to task?
- Mass flow or mass per batch of each material leaving the task?
- Volume flow or volume per batch of each material fed to task?
- Volume flow or volume per batch of each material leaving the task?
- Do volumes and/or densities change significantly during the task?
- Residence time in the task to allow desired process to occur? (note: different residence times might be required for each phase)

Mixing

- Bulk mixing time required? (for stirred tanks or similar)
- Micromixing time required? (or could be expressed as energy dissipation/volume)
- Method of introduction of fed phase(s)?
- Phase dispersion? (e.g. solids suspension, dispersion of one liquid phase in another, gas dispersion in liquid)
- Influence of process material properties? (e.g. high viscosity)
- Variability of mixing requirement? (e.g. does mixing need to be more intensive during one part of a task compared with another?)

Energy transfer

Links to residence time, mass transfer, maximum permissible temperature

- Form of energy to be transferred? (heat, ultraviolet light, microwave etc.)
- Quantity of energy to be transferred?
- Heat transfer intensity requirement? (UA/V will be relevant to exothermic reactions etc.)
- Heat transfer as a ratio to mass transfer (UA/K_La or similar will be relevant to mass-transfer-limited exothermic reactions etc.)

- Variability of heat transfer requirement? (e.g. in second-order plug-flow exothermic reaction)

Mass transfer

Links to phase and flow characteristics

- Interphase mass transfer requirement? (G-L, L-L, L-S etc.)
- Mass transfer intensity requirement? ($K_L a$ or similar)
- Specific surface area required? (for quasi-instantaneous two-phase reactions)

Phase and flow characteristics

- Phases present in materials entering the task?
- Phases present during the task?
- Phases present in materials leaving the task?
- Particle, droplet or bubble size distribution?
- Phase ratios? How do phase ratios change with task progress?
- Required contacting pattern? (co-, cross- or counter-current)
- Which phase must be dispersed, which must be continuous?
- Is phase inversion possible? Should it be avoided or encouraged?
- Is phase separation required?
- Does relative density of phases change? If so, what are the implications?

Physical processing conditions

- Shear and elongation required to break droplets in a liquid-liquid system?
- Other shear requirement?
- Compression?
- Impact?

Operability

- Maximum temperature permitted?
- Minimum temperature permitted?
- Pressure capability?
- Materials of construction?
- Cleanability requirements?
- cGMP capability?
- Start-up and shut-down provisions?
- Sampling?
- Special inerting?

Other

- Other items, specific to this task?
- Items relating to interfaces to earlier or later tasks?