# Equipment selection within the IMPULSE Multiscale Process Design framework

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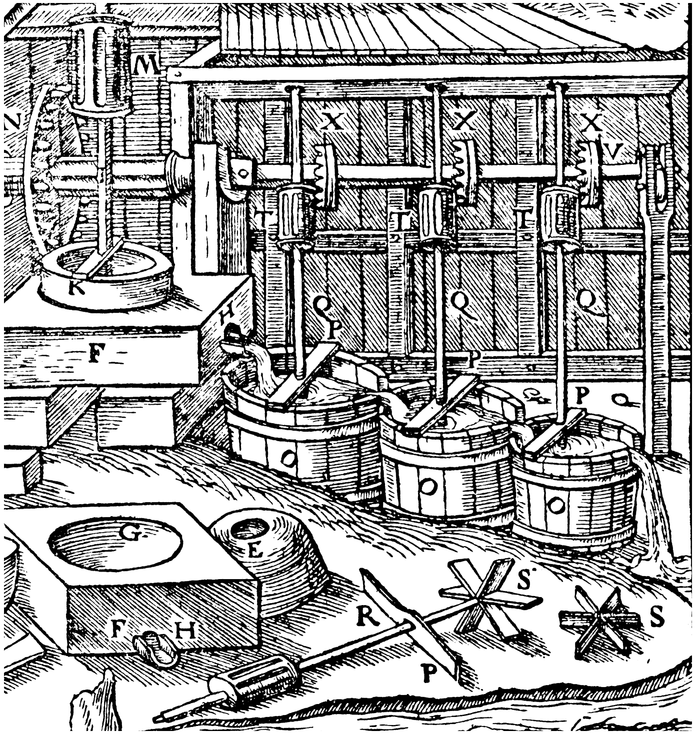
# Introduction

- Structure of presentation
  - Introduction and context
  - Development method
  - Approach
  - Mapping process tasks to equipment
  - Technology Option Identification Methodology (TOIM)
  - Equipment Database
  - Conclusions

# The industrial context

- Low tonnage chemicals are usually made by batch processing
- Continuous processes are only considered if a batch process is too difficult
- Chemical engineers and chemists in the batch industry are often not familiar with continuous processes and equipment
- Thus equipment is often predetermined
- The IMPULSE team hopes to change this...

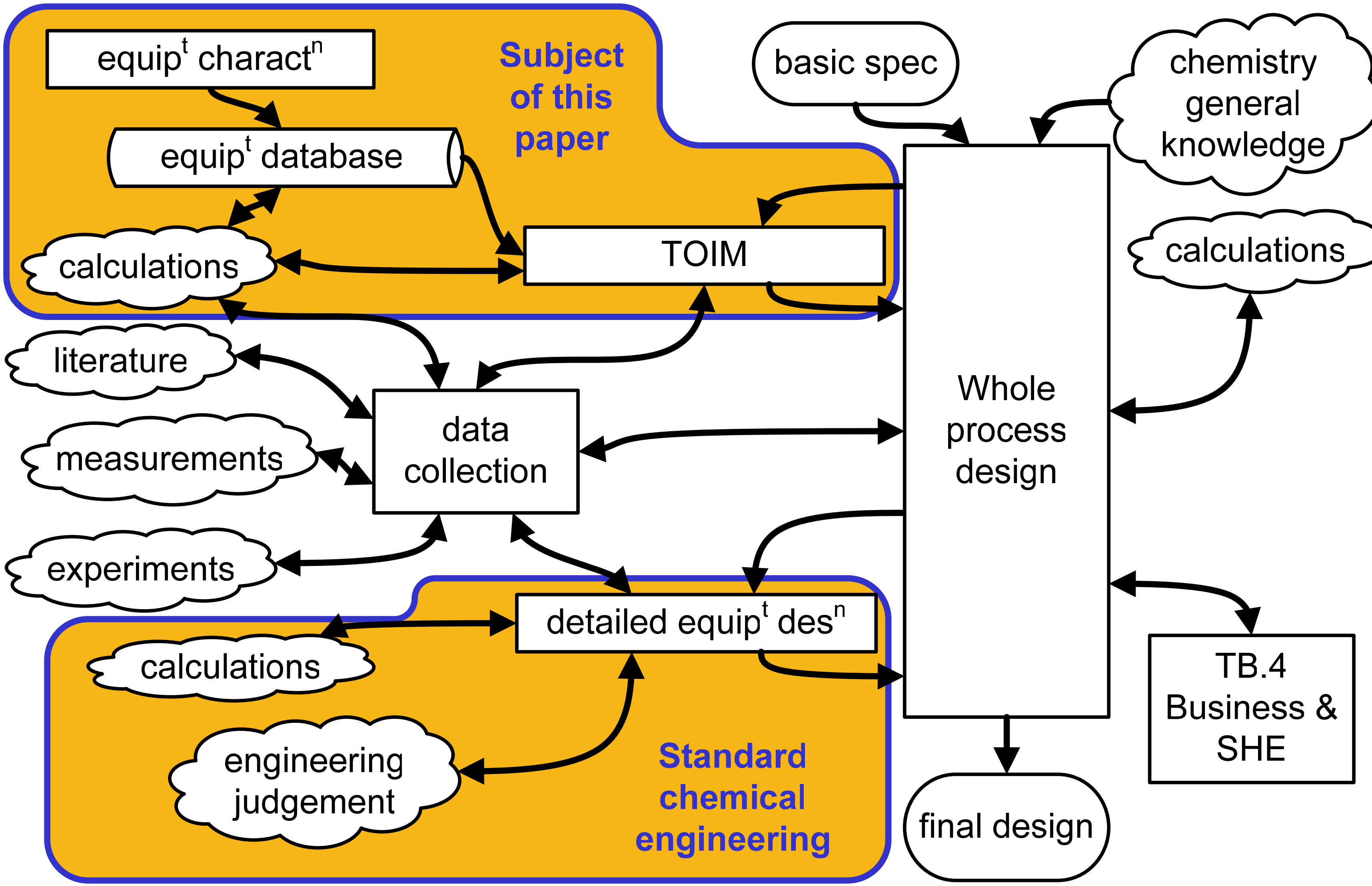



Georgius Agricola,
*De Re Metallica*, 1556.

# Technology Option Identification — Aim

- At the end of IMPULSE, we want to have a **methodology** to help the designer select the **best technology option** for a particular process need, using structure of an **appropriate scale**
- To do this, we need:
  1. standard methods for characterising equipment
  2. a database of equipment
  3. methods for characterising processes to identify equipment needs
  4. a software tool that finds equipment in the database that would meet the process need

# Technology Option Identification in context



# Development method

- Collaborative work by experts from
  - Britest and its member organisations
  - Forschungszentrum Karlsruhe (FZK)
  - Institut für Mikrotechnik Mainz (IMM)
  - CNRS-LGC, Toulouse
  - University of Manchester
- Brainstorming, prototype methods, feedback, revision
- Methods are based on the underlying science and the practical experience of the team

# Approach

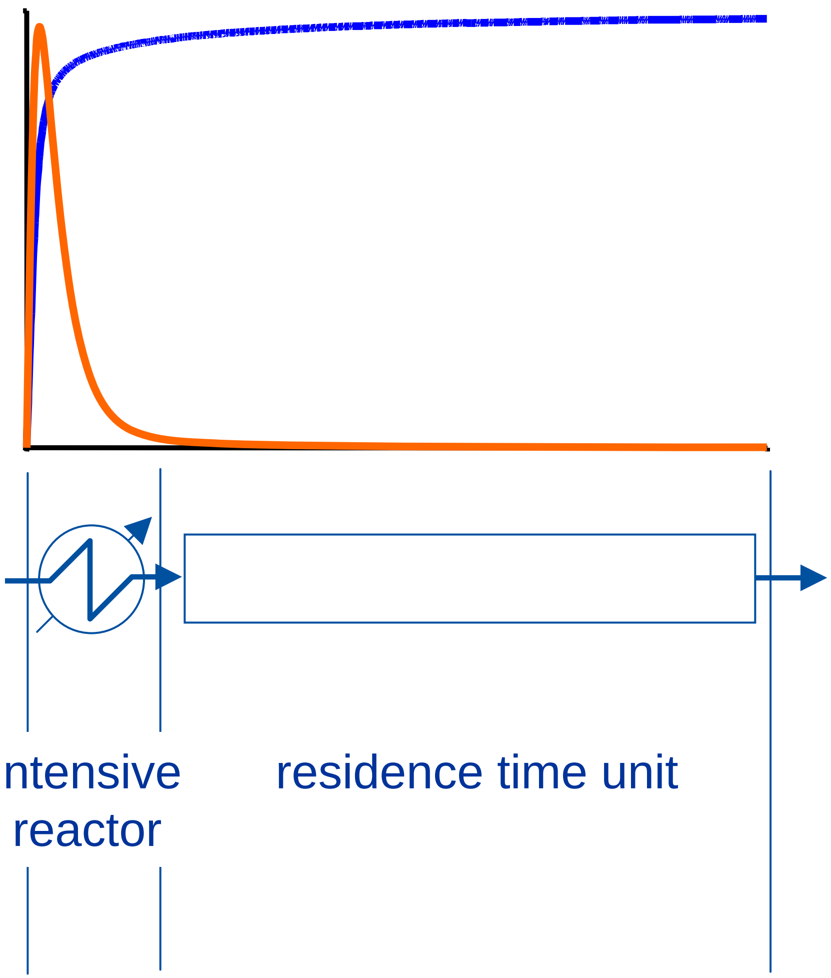
1. Understand the process in terms of the fundamental physics and chemistry
   - reactions, desired and undesired
   - phases, mixing etc.
   - rate determining phenomenon?
   - qualitative; quantitative where necessary
2. From this process understanding, define what the process needs the equipment to deliver
   - residence time, mass & heat transfer etc.
3. Find equipment that can meet these needs
   - database of equipment characteristics
   - searching methodology

# Mapping process tasks to equipment

- A process is a sequence of tasks carried out to transform feedstocks into desired products
- The whole process might better meet the business needs if:
  - some tasks were combined in a single item of equipment; or
  - some individual tasks were split among two or more items of equipment in series
- So the mapping of tasks to equipment is important for the viability of the whole process

# Splitting tasks

- 2nd order reaction in plug flow reactor
- High reaction rate and heat output in first 10% of reactor volume
- Much lower heat transfer requirement in remaining volume
- Splitting the reaction task between two equipment items gives a cheaper overall process



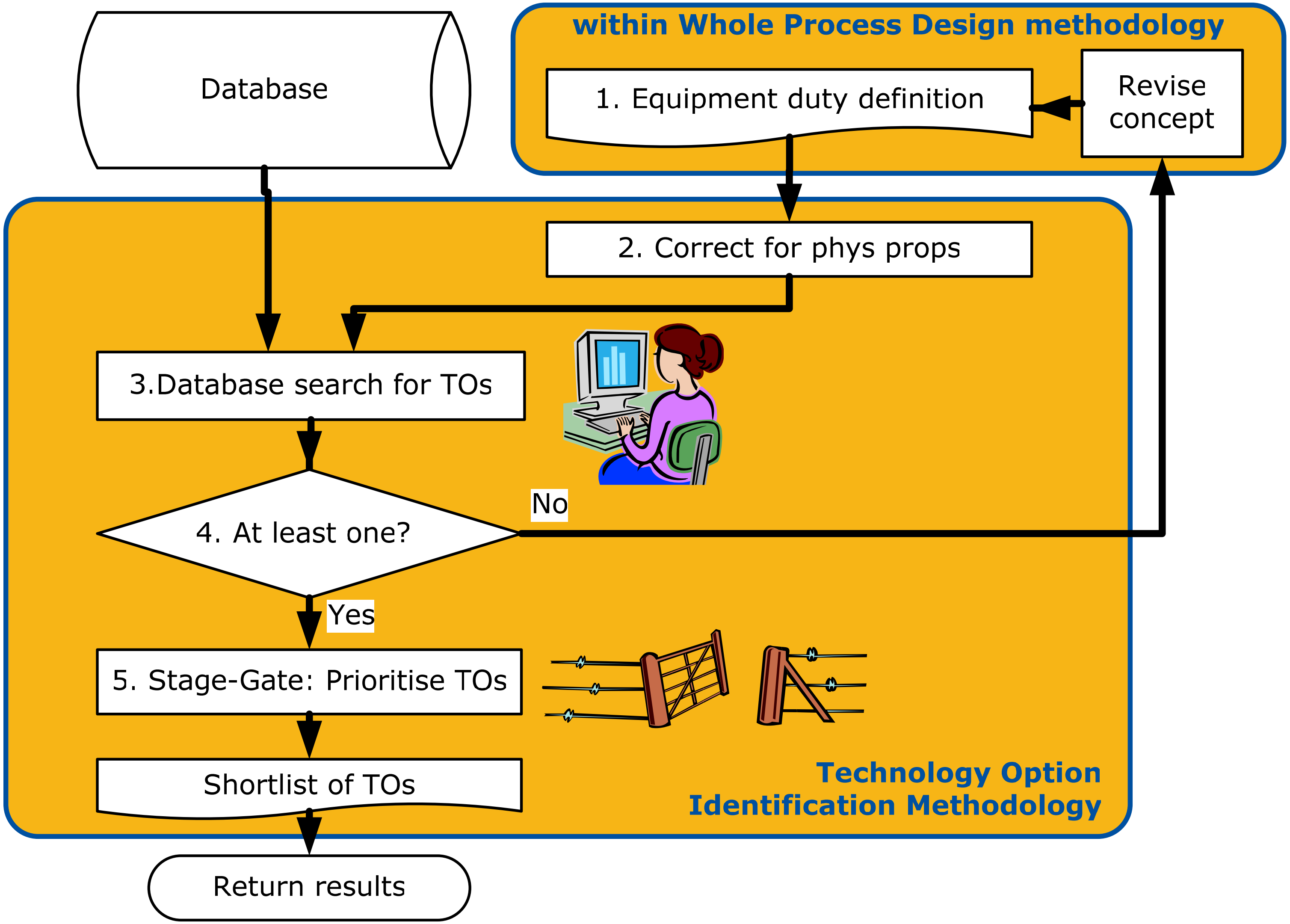
# Splitting tasks

- General principle for splitting tasks:
  - Splitting of a task should be considered where the required duty varies widely as the task progresses

# Combining tasks

- When deciding whether to consider combining tasks all these criteria should be met:
  1. the materials present in all of the tasks to be combined should be compatible with each other,
  2. the required processing conditions should be similar, and
  3. the duties required of the equipment should be similar
- If duties or processing conditions for the tasks being combined are too far apart, the resulting compromises lead to a higher overall cost

# TOIM


within Whole Process Design methodology
Database
1. Equipment duty definition
Revise concept
2. Correct for phys props
3.Database search for TOs
4. At least one?
No
Yes
5. Stage-Gate: Prioritise TOs
Shortlist of TOs
Return results
Technology Option
Identification Methodology

# Equipment characteristics

- What characteristics of equipment will allow selection of the best technology option to meet a process need?
- Characteristics must be:
  - related to the process needs (duties)
  - measurable using cheap, safe tests
- A list of characteristics was developed
  - to facilitate the equipment duty definition
  - to define the characteristics of equipment that must be measured
  - to provide a structure for the equipment database

# Equipment characteristics

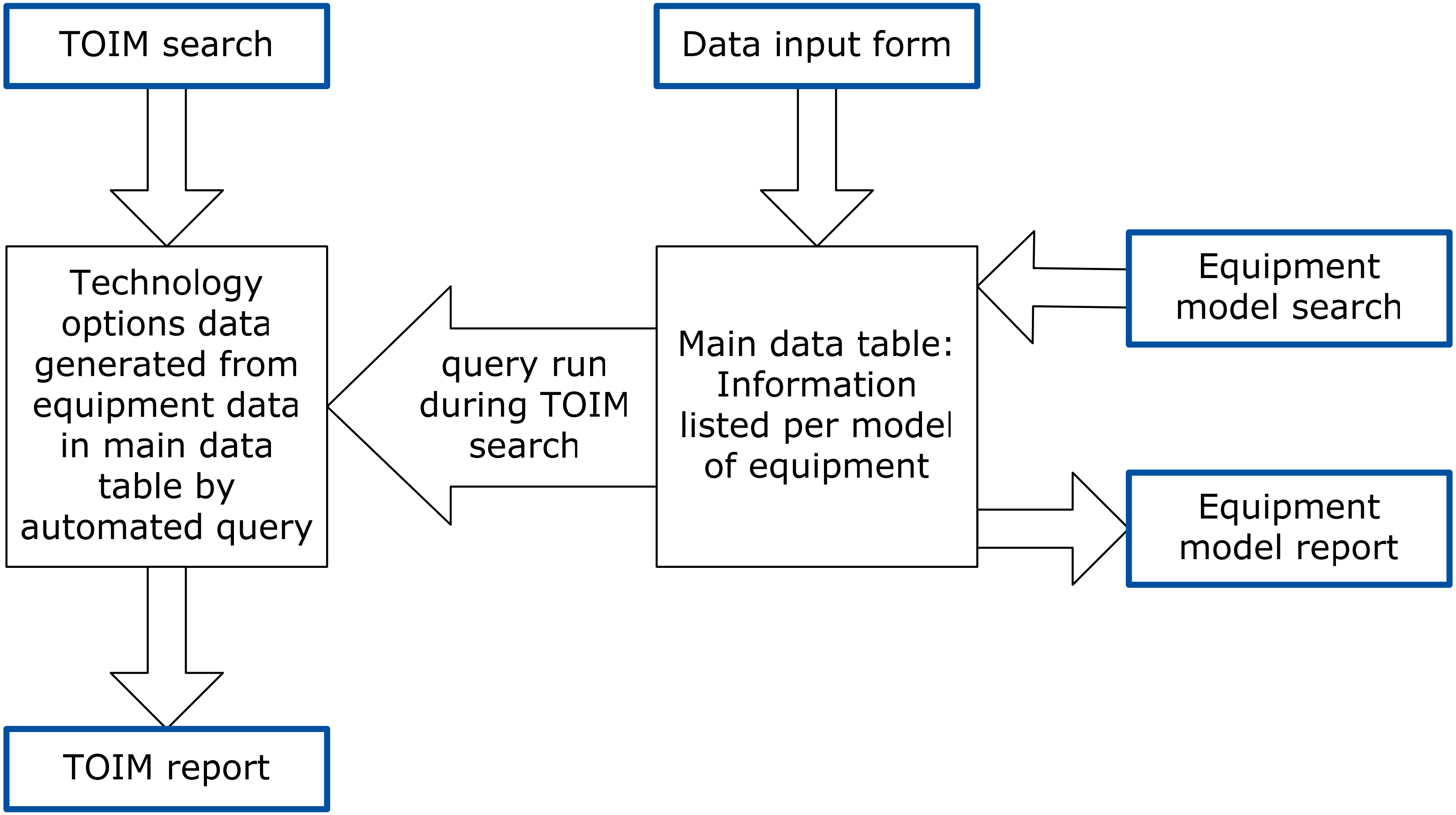
| | | | |
|---|---|---|---|
| 01 | | **Equipment name** | |
| 02 | | **Unique identifier** | |

| | | | |
|---|---|---|---|
| | | **Material balance & residence time** | |
| 03 | * | Total mass flow into the device | Range, kg/s |
| 04 | * | Volume | Range, $m^3$ |
| 05 | * | Residence time gas | Order of magnitude range, s |
| 06 | * | Residence time light liquid | Order of magnitude range, s |
| 07 | * | Residence time heavy liquid | Order of magnitude range, s |
| 08 | * | Residence time solid | Order of magnitude range, s |

| | | | |
|---|---|---|---|
| | | **Mixing** | |
| 09 | * | Bulk mixing time to achieve 95% mixing, $t_{95}$ | Order of magnitude range, s |
| 10 | * | Micromixing characteristic mixing time | Order of magnitude range, s |

***etc…***

# Database structure



# Database status

- Structure and searching method is complete
  - some tweaks may be needed in the light of experience
- More data are needed to populate the database
  - please contact Jeremy Double if you would like to help
  - a form and instructions will be provided

# Simple example

- Single-liquid-phase reactor with heat transfer duty and no other special requirements
  - reaction time 10 minutes
  - throughput of 24 L/min
  - heat evolution of 20 kW
  - 20°C temperature difference available
  - process fluids are water-like
    - no adjustment for physical properties
- Required volume
  - throughput × reaction time
  - 24 L/min × 10 min = 240 L = 0.24 $m^3$

# Example part 2

- To look at the heat transfer capability, use the heat transfer intensity parameter, *UA/V*

$$Q = U\ A\ \Delta T$$

so

$$\frac{U\ A}{V} = \frac{Q}{\Delta T\ V} = \frac{20000\,\mathrm{W}}{20\,\mathrm{K} \times 0.240\,\mathrm{m}^3} = 4167\,\mathrm{W/\ K\ m}^3$$

- batch stirred tank ~700 W/K $m^3$ not OK
- tubular reactor ~70 000 W/K $m^3$ OK
- microreactor ~5 × $10^7$ W/K $m^3$ OK

# Conclusions

- By providing a structured approach to equipment characterisation based on:
  1. a consideration of process needs
  2. a set of standard tests for making measurements according to this approach
  3. a database tool for recording the characteristics of each type of equipment

  rapid shortlisting of appropriate process equipment will be facilitated

  - thus making process development quicker and more effective

# FP7 PILLS Project