



Innovation Appraisal Group * Gideon Samid, PhD

Chemical Engineering Series

Reactor Design (classic)

Innovative Chemical Engineering

Pf. Gideon Samid, PhD, Head, Innovation Appraisal Group,
Phone: 571.214.9814. gideon.samid@CASE.edu

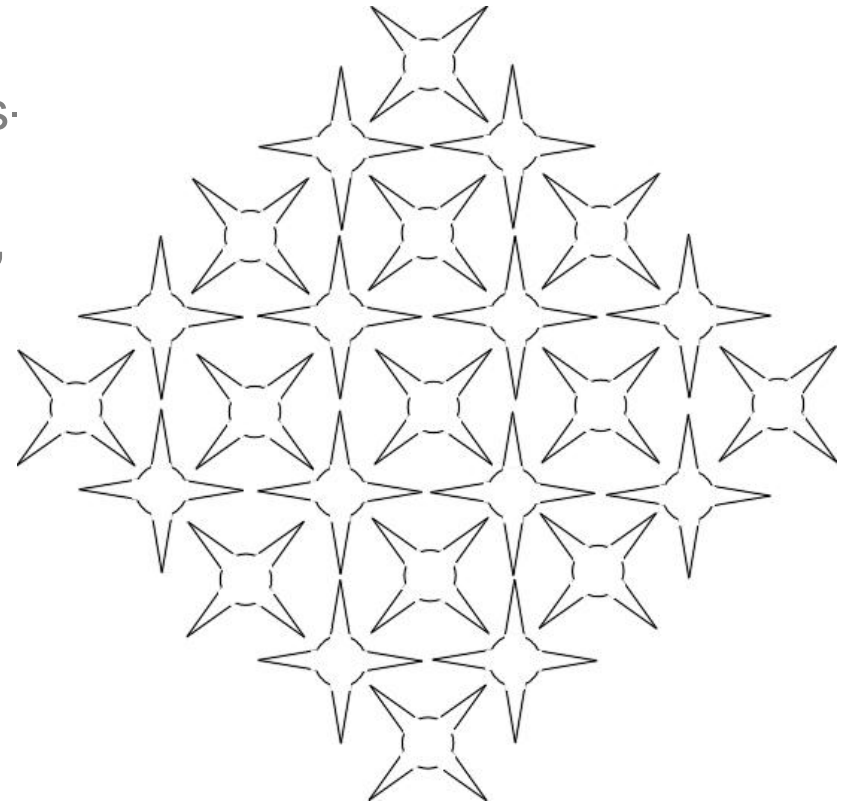
Plant's Center point

- An industrial chemical plant is a reactor, where the reaction of reference takes place plus everything that feeds to it, and disposes of its output.
- It's where the reactants come into intimate contact subject to the right conditions (physical, chemical).



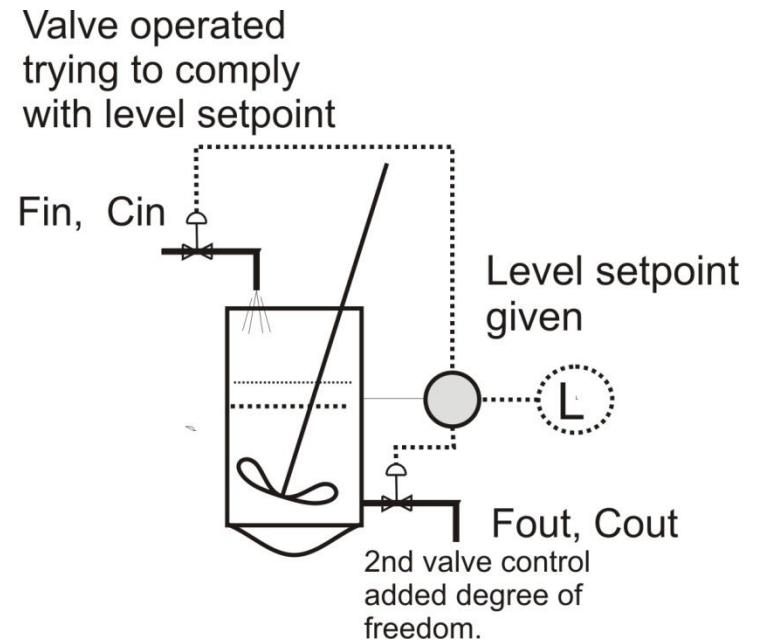
Reactors' Types

- Batch v. continuous
- bubble columns, slurry reactors, gas-solid fluidized beds, catalytically structured reactors, distillation trays, catalyst containing trays, ..
- Classical (mixed vessel), pipe-reactors, collision-reactors...
- Durables, temporary, transients...



Classic Reactor

- Stirred container
- One or more inlets, one or more outlets
- Heating/cooling facilitation
- Instrumentation & control
- Pressure/Vacuum options.



Classic Design Questions

- Volume, Material of Construction, pipes spec – case dependent
- Shape, mixer, heat-exchange, support, instrumentation, maintenance, safety – standardized



Volume (single)

- **Single Continuous:**

Parameters: Production Capacity (Q), hours of use per day (h), reaction time (T)

$$q = \frac{Q}{h} \quad V = qT$$

- **Single Batch:**

Parameters: Q, h, preparation time, T_p , cleaning time, T_c :

$$q(T_p + T + T_c) = V$$

Volume (multiple)

- **Continuous: n variable sizes:**

Combine available sizes to satisfy summation:

$$V = \sum_n V_i$$

- **Batch:**

Lines overlap:

$$V = \mu \sum_n q_i (Tp_i + T_i + Tc_i)$$

$$q = \sum_n q_i$$

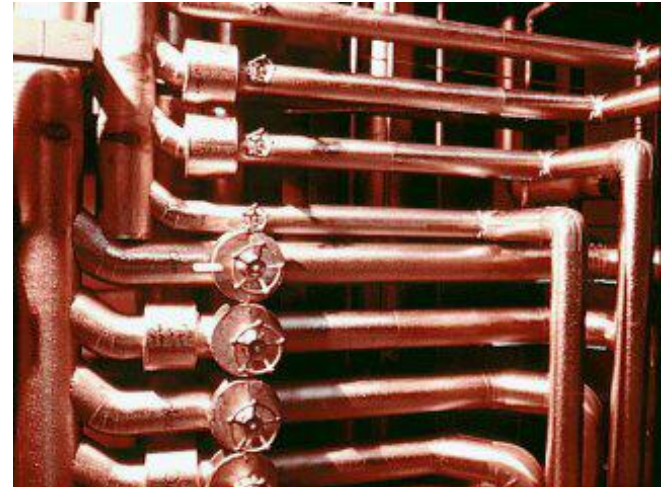
Modern Classic Reactors

- Re-Use of standardized vessels.
- Electric Heating option
- Premium mixer design
- Configuration options design



Heating/Cooling

- Apply to inlets, or to reactor per se?
- Inserted source, or a walled option?
- Selecting the most available energy source: air, water, steam
- Compute energy balance generously: allow for environmental loss, surface deterioration on both sides, material spec. fluctuations.
- Safety scenario: leakage, contact



Mixing

- Standard reactor calculation assumption:
 1. instant mixing
 2. temperature step function
 3. average reactor time = actual reactor time.
- Reality:

Mixing zone variance, leading to interim temperature pockets, allowing some feedstock to leave reactor prematurely, while some feedstock is trapped for a prolong stay.

One woman ninth month pregnant is on average the same as nine women first month pregnant.

Mixer Design

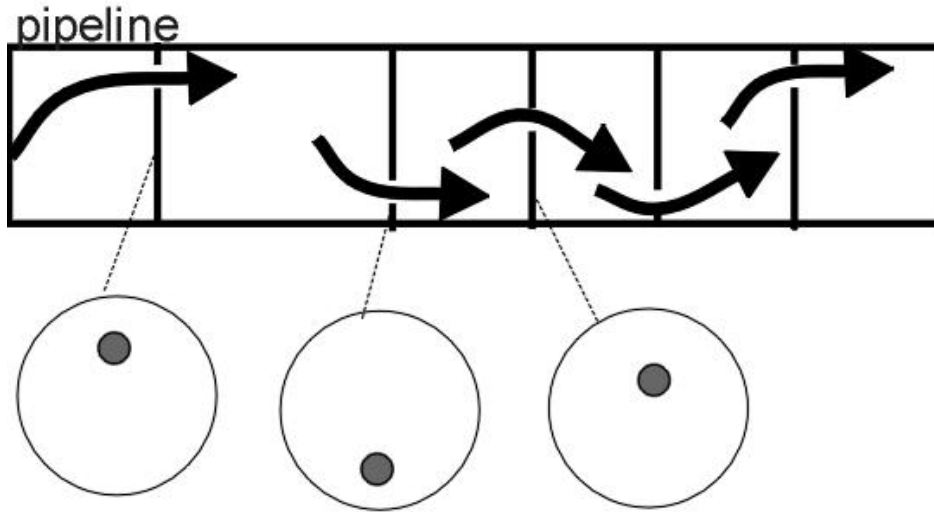


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- Impellers/Baffles
- Kneaders/Dispersers/Masticators
- Tumbling Mills
- “Mix-Fix”
- Heat Release/Viscosity changes/Material damage consideration.
- Energy Requirements.
- Serial Mix Configuration.

Mix-Fix (no moving parts)

MixFix

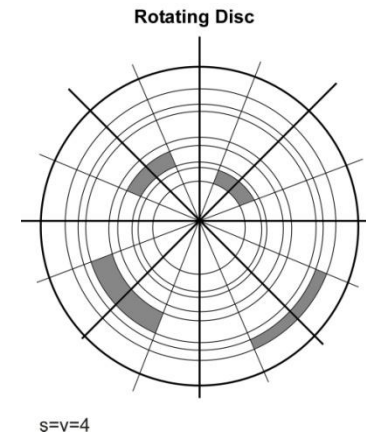
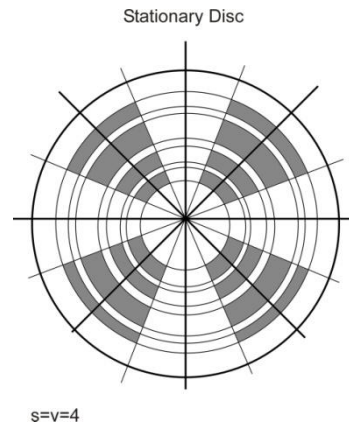
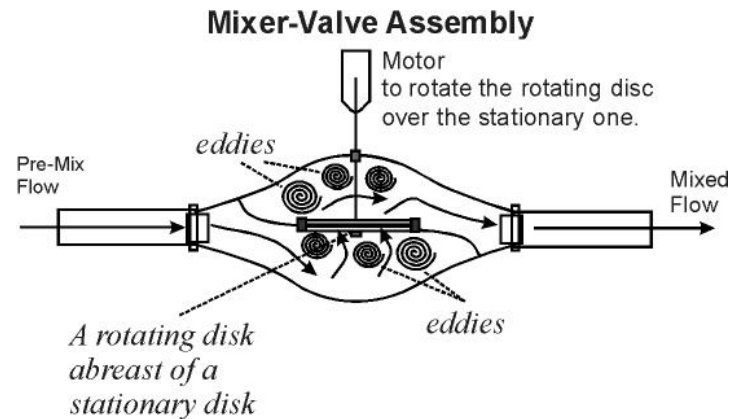


The shaded area represents the hole in the disc. The fluid in the pipeline must bend its streamlines to flow through each hole.

The arrows depict fluid flow
discs
with mismatched holes
create turbulence

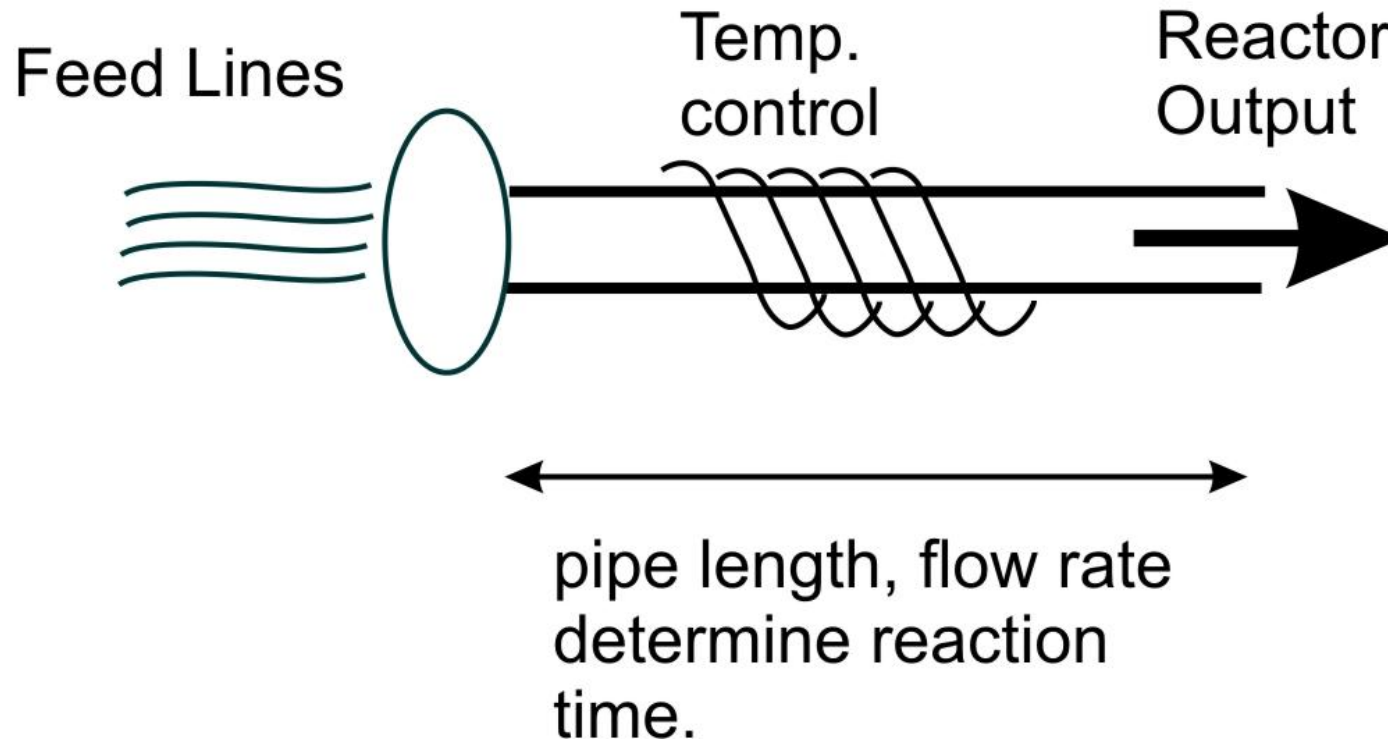
Mix-Fix (main)

- No off-average variance
- Mixing degree tightly controlled
- Doubles as valve



Pipe Reactor

Pipe Reactor (Mix-Fix)



Viscosity

- It changes with temperature.
- It changes with pressure.
- It changes with degree of mixing
- It often changes with force and speed gradient

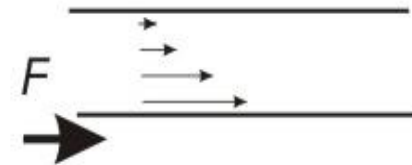
Fluid Motion

* as bulk



F works against wall friction, and mass resistance of fluid.
(Pumping)

* as layers



F moves one plate, creates a velocity gradient vs. the stationary plate

$$F/A = \mu (dv/dy)$$

μ - viscosity, typical of fluids.

If Viscosity independent of F . (dv/dy) then Newtonian.

Viscochallenge

- Viscosity resists mixing, resists heat transfer.
- Mixing changes viscosity, releases heat.
- Mixing, viscosity, exothermic/endothermic reactions – a perfect viscochallenge.
- Handle:
- *acquire derivative pair data ($dx1/dx2$) $x3,x4,\dots$*
- *Consider serial configuration simplification*
- *Mathematical modeling*
- *Design reserve capacity: pumping power, mixing power, heat-exchange*
- *Pilot Plant.*

Mixing Illustration (1)

- A veterinary pill was to be a mixture of seven ingredients. The chemist and the vet who developed the formula administered the ingredients separately, and assumed it would be a simple engineering challenge to premix the components. Alas, it turned out that for the ingredient mix to be fluid it had to be heated to about 200F. However two of the ingredients were mutually reactive at that temperature. The engineers tried for several weeks to tinker with the mixing challenge, and failed. When they lowered the temperature to prevent a reaction, the viscosity climbed up, and the mixing became ineffective. The chemist tried to solve the difficulty his way by searching for a de-catalytic ingredient that would hinder the reaction. The working solution was not mentioned because it was too expensive... The only way to insure proper mixing was to mix the first six ingredients with the 7th one in a powder form.

Batch Reactor Mixing



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- First pour ingredients, then mix?
- Pour one ingredient, mix while pouring the other?
- Pour all ingredients while mixing?
- Considerations: **viscosity, temperature, mixing efficiency.**

configuration



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- **Parallel reactors** (smaller, operational flexibility – maintenance, accidents, re-use)
- **Serial reactors** (mixing stages, subsequent ingredient add on).
- Combination

Heat Exchange



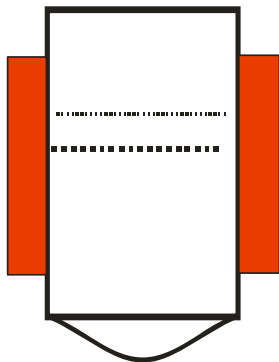
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- **Classic**: fluid-to-fluid:
 - direct contact (ready separation)
 - walled contact (*nominal*)
- **Special**: fluidized bed, electro-heating, electromagnetic heating, sound-waves, mechanical conversion

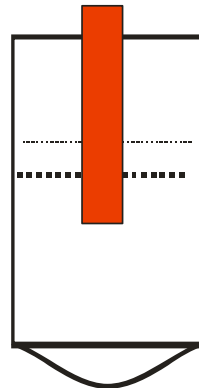
Walled Contact Heat Exchange

Heat Exchange Options

External Wall



Internal Element



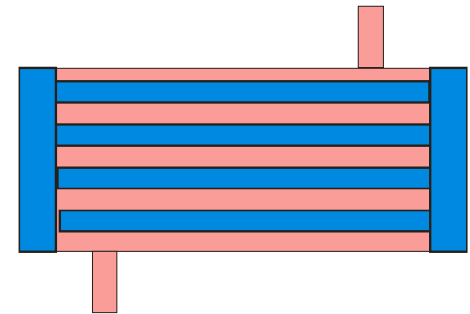
Pipeline Heat Exchange



Pipeline heating:
better surface to
volume ratio, may
need longer
pipeline, more
pumping energy.
Mixer evens out the
temperature
throughout the
reactor. Changing
pipe, easier
maintenance.

Pipelined Exchange

- Concentric tubes
- Tubes & Shell
- Parallel Plates
- One/Several passes
- Parallel Flow/Counter-Parallel
- Exchange Efficiency vs. Maintenance Efficiency (tube diameter).



Heat Exchange Computation

- Heat flow ΔQ , is proportional to ΔT per each point of heat flow.
- ΔT changes along the exchange route per:
 - *heat capacity of both fluids*
 - *flow rate of both fluids*
 - *flow regimen of both fluids (turbulence)*
 - *effective exchange area*
 - *wall quality*
- ΔT changes over time per wall scaling, rusting, staining.

Basic Heat Exchange Math

Assuming no heat loss: all energy lost by hot fluid is gained by the cold one.

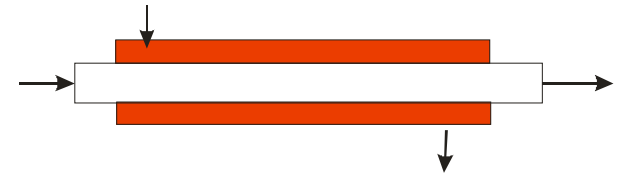
Each fluid sustains a temp. change determined by its heat capacity, and flow rate:

$$K(Th - Tc) = Ch * Qh * (dTh/dx)$$

$$= Cc * Qc * (dTc/dx)$$

Resolving to:

$$Th = A - B e^{-kx} ; Tc = A' + B' e^{-k'x}$$



$$Th(mean) = \int Th(x) dx$$

$$Tc(mean) = \int Tc(x) dx$$

$$LMTD = Th(mean) - Tc(mean)$$

$$\Delta Q/\Delta T = K * L * (LMTD)$$

In Series Exchangers

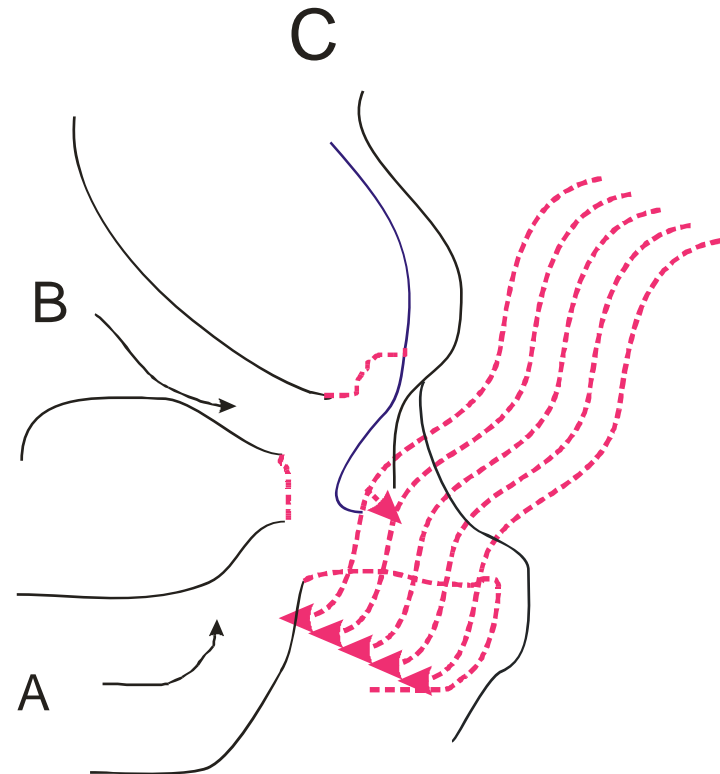


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- Option to standardize
- More powerful control
- Easier maintenance
- Greater cooling/heating fluid options.
- Smaller size (easier handling)
- Overcapacity: more freedom of flow-rates, pumping head.

Exotic Exchangers

- Electromagnetic transfer of energy, engineered to induce flow, mixing, compounding.



Reactor Design Perspective

- Not typically the most expensive part, but it determines the most expensive parts (pumps, heat exchangers, storage tanks, civil, control).
- *A rough reactor design is a good design start!*



Seminar Offerings



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- Engineering is Cost Engineering
- Chemical Engineering for Innovative Chemistry
- Innovation Acceleration Methodologies
- The Universal Theory of Innovation
- Innovation Management
- BiPSA: Management by Inclusion
- Nurturing the Culture of Innovation

Seminars range from a single evening overview, a dedicated Saturday; six, ten, and thirty hours on a weekly or bi-weekly basis, and per-case arrangements.

Seminars are offered (1) online, (2) at Case Western Reserve University, (3) on the road, (4) on customer's location.

Contact:

Shennan L. Madden, Department Secretary
Case Western Reserve University
Chemical Engineering Department
A.W. Smith Building, Room 116, 10900 Euclid Avenue
Cleveland, OH 44106-7217
(216) 368-4182 (voice) (216) 368-3016 (fax) slm33@case.edu

Gideon Samid, PhD, Head, Innovation Appraisal Group
Pf. [Adj.] Department of Chemical Engineering
School of Engineering, Case Western Reserve University
A.W. Smith Building, Room 116, 10900 Euclid Avenue
Cleveland, OH 44106-7217
(571) 214-9814 (voice) gideon.samid@case.edu