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The Concept of Chemical Similarity for Optimization and Design of Gas-Solid Processes

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Contents:

- **The Principal Problems in Chemical Engineering**
- **Industrial-scale Processes**
- **Advantages/Disadvantages of Lab-scale Units**
- **Laboratory-scale <=> Industrial-scale**
- The Traditional Approach
- The Concept of Chemical Similarity
- Example:
- **The Importance of Radicals**
- From the Single Particle to the Pilot-scale

Principal Problems in Chemical Engineering

- **Reactor/Process Design?**
- **Operating Conditions?**

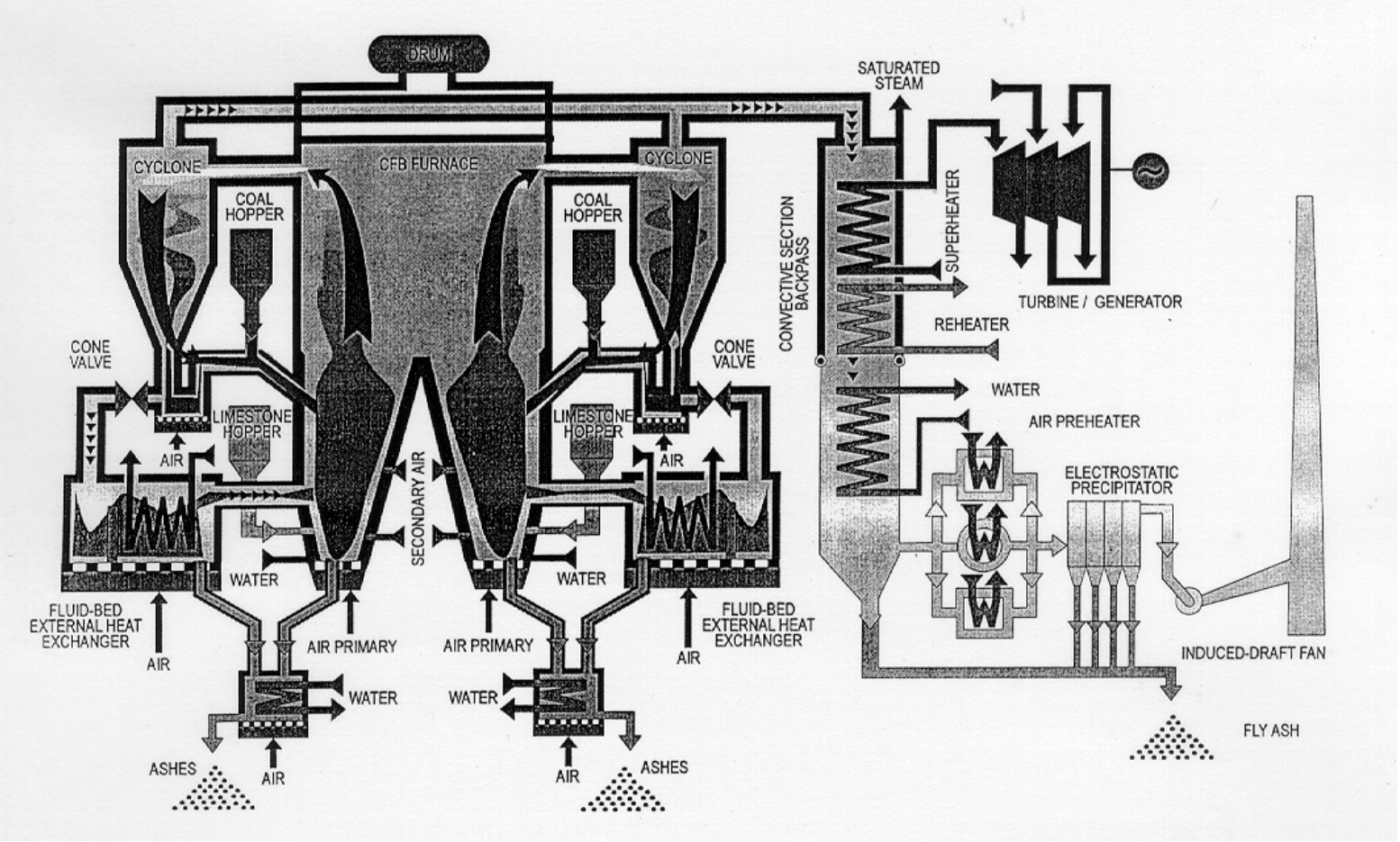
to achieve:

- **High Productivity!**
- **High Quality!**

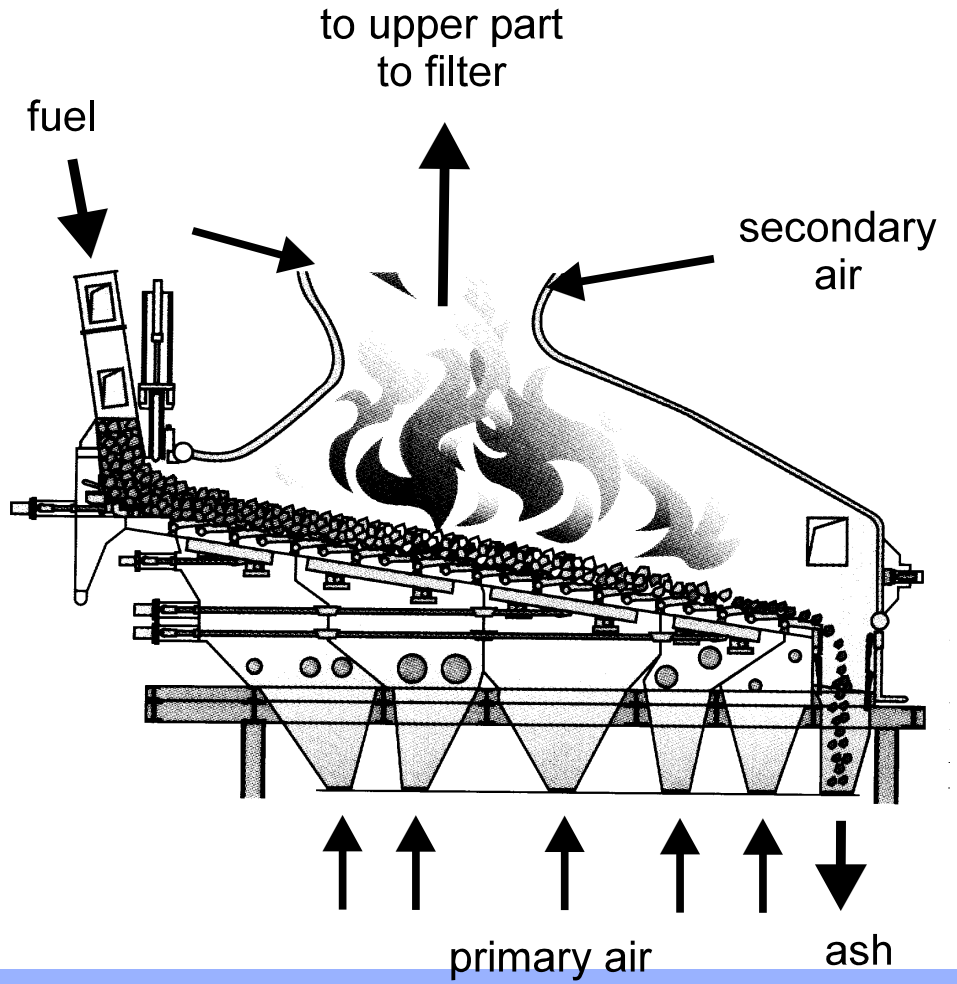
at

- **Clean Environment**
- **Low Costs**
- **Short Time**

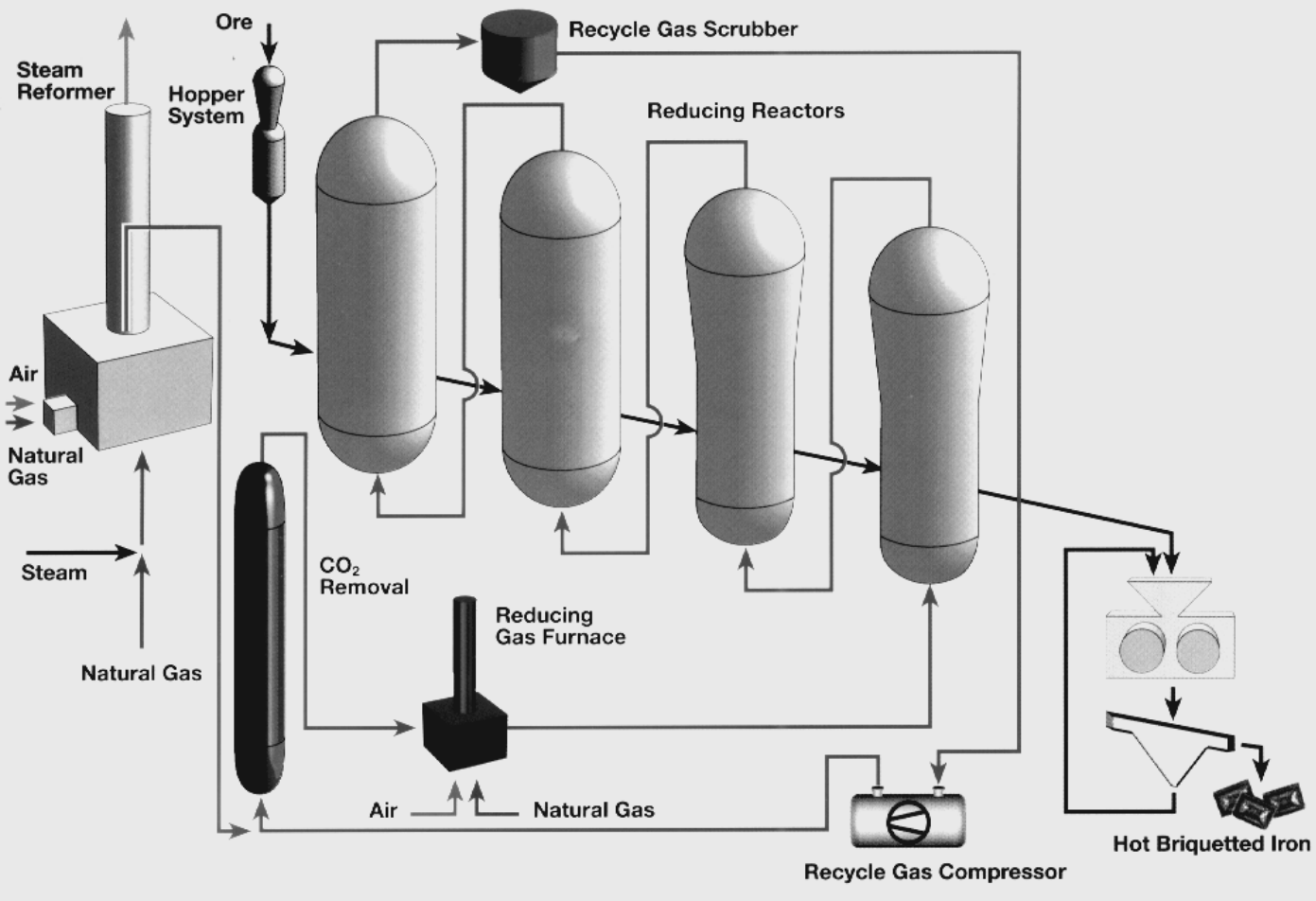
Industrial-scale Processes - Fluidized Bed Combustion



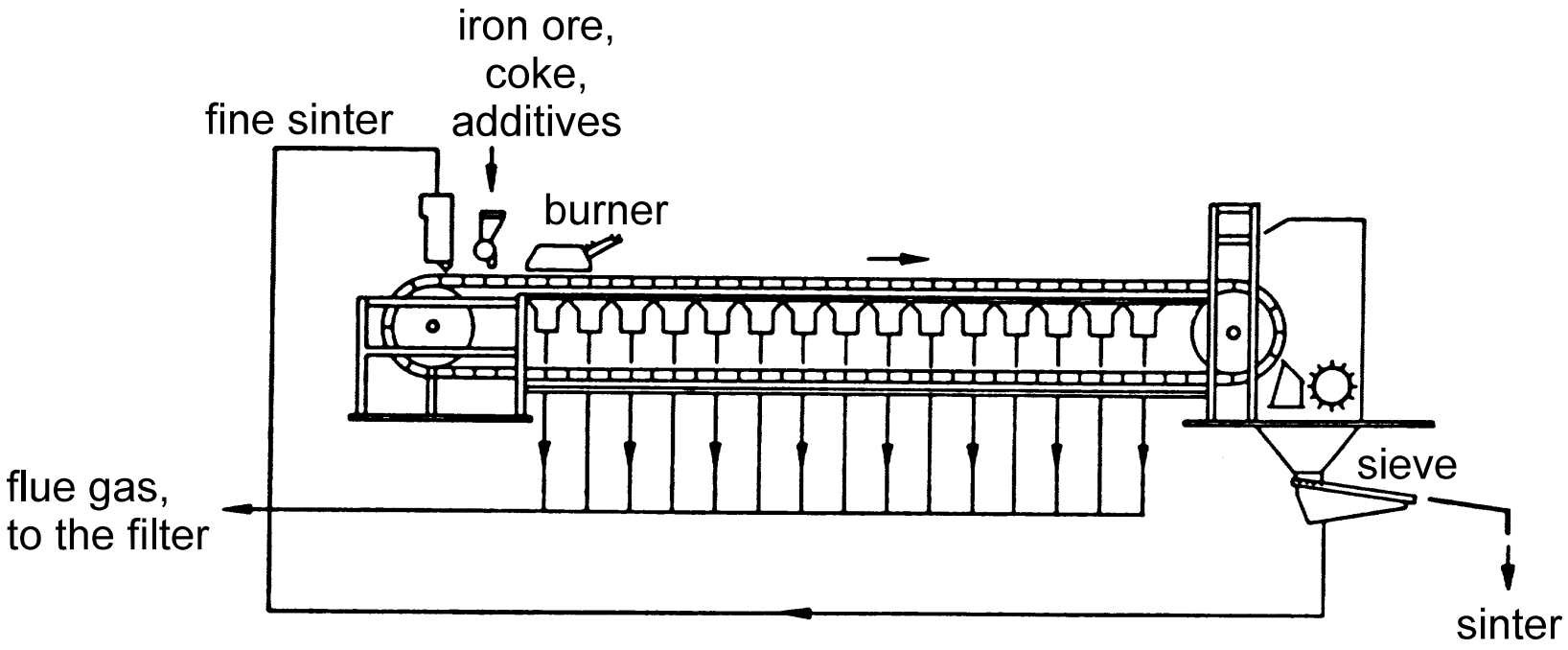
Industrial-scale Processes - Grate Combustion



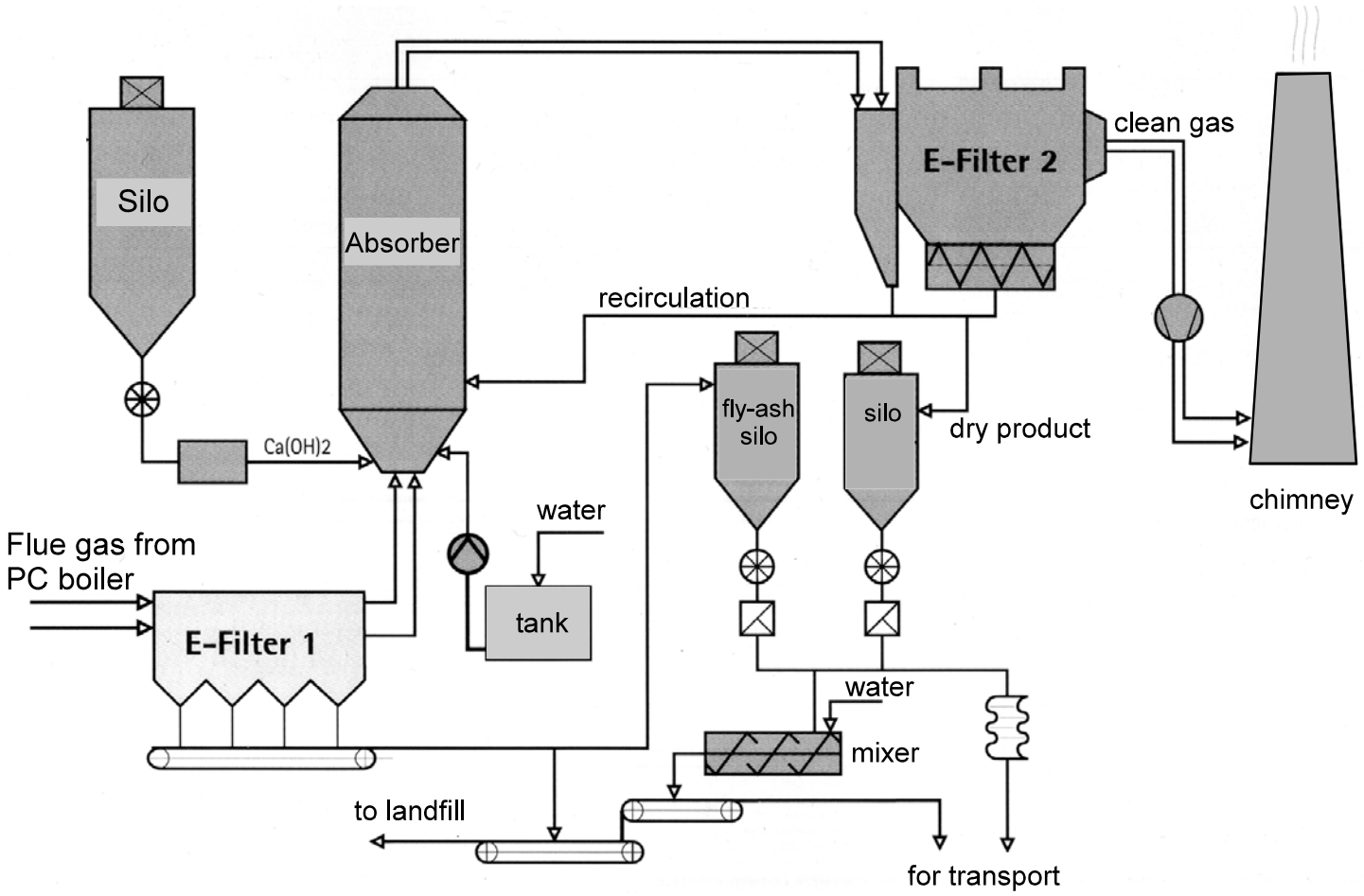
Industrial-scale Processes - Iron Ore Reduction



Industrial-scale Processes - Iron Ore Sintering



Industrial-scale Processes - Flue Gas Desulfurization



Industrial-scale Processes - Conditions

	Combustion			Iron Ore Reduction	Sinter Process	De-sulfurization
techn.	fixed	fluidized	entrained	fluidized	fixed	fluidized
gaseous reactants	O_2 (air)	O_2 (air)	O_2 (air)	H_2, CO, CH_4	O_2 (air)	SO_2, CO_2, HCl
solids' temp.	400-1000	600-950	900-1700	600-900	800-1400	60-150
pressure	atmos	1-17	atmos	~11	atmos	atmos
sup. gas velocity	1-4	1-2.5 3-8	5-10	~1	1 (cold)	1-5
solid reactants	biomass, waste	coals, biomass, waste, sludge	coals, co-comb. with biomass	iron ore	cokes, alternative fuels, met. waste	$Ca(OH)_2$

Industrial-scale Processes - Conditions

	Combustion			Iron Ore Reduction	Sinter Process	De-sulfurization
tech-nology	fixed	fluidized	entrained	fluidized	fixed	fluidized
particle size	10-100	1-30 0.5-10	0.010-0.100	0.05-6	0.2-5 (cokes)	0.001-0.01
heating rates	low	medium - high	very high	medium - high	high	low
lab-scale methods	- TGA - fixed bed	-fluid. bed (bubb., circ.)	-entrained -burners -grid heaters -matrix react.	- fluidized bed - fixed bed	-fixed bed - fluidized bed	- TGA - fluidized bed (circulating)

Laboratory-Scale Units

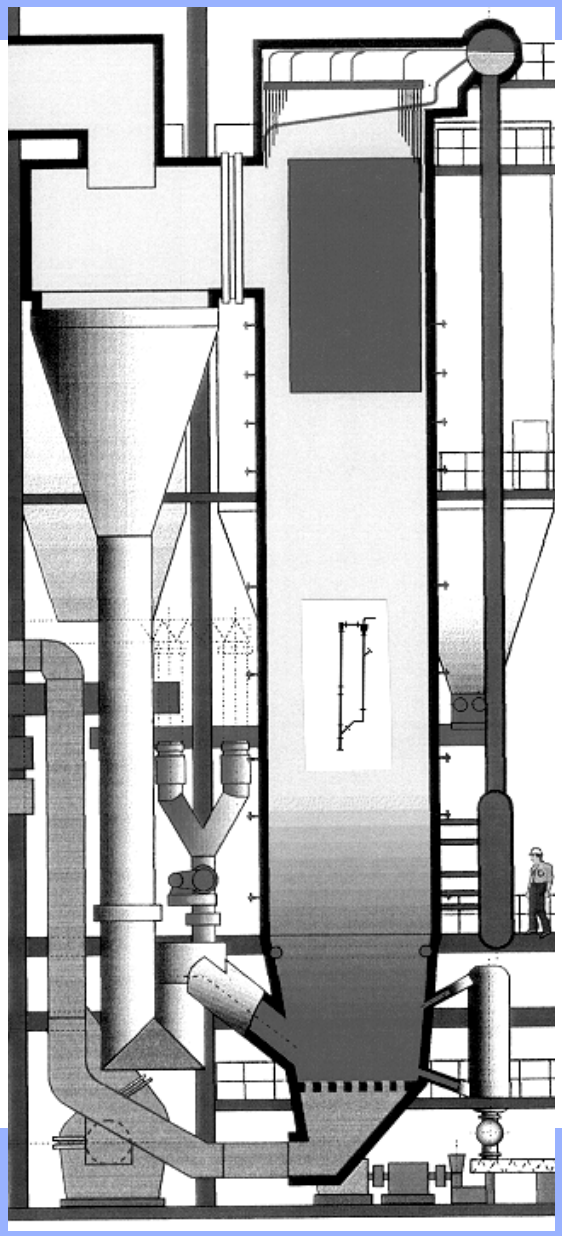
ADVANTAGES:

- inexpensive
- low operation costs
- high availability
- design changes - quickly & low cost
- operating conditions - broad range
- good instrumentation

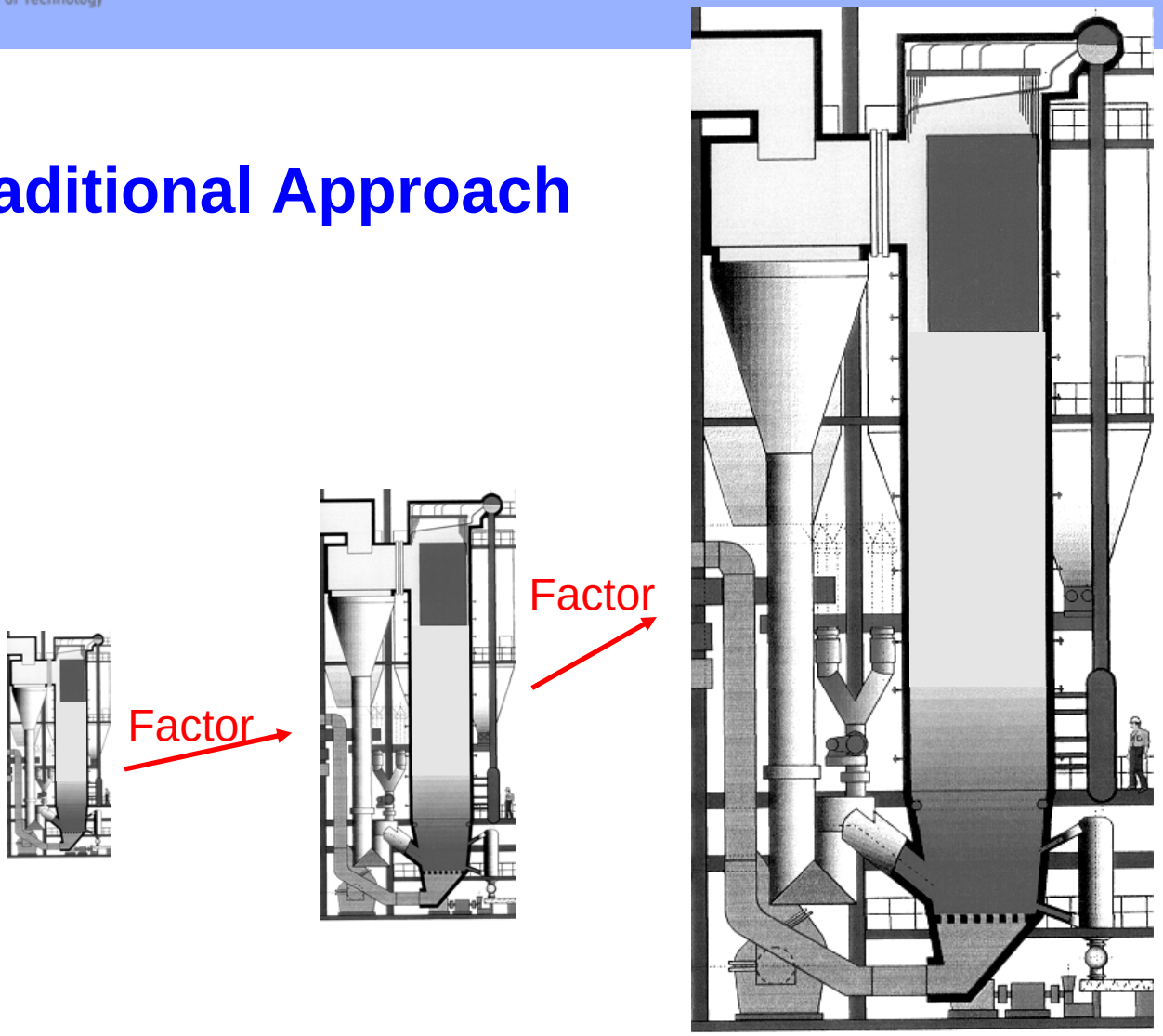
DISADVANTAGES:

- **uncertainty to transfer results to industrial-scale units**

Comparison between Laboratory-scale & Industrial-scale Units



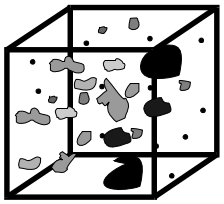
The Traditional Approach



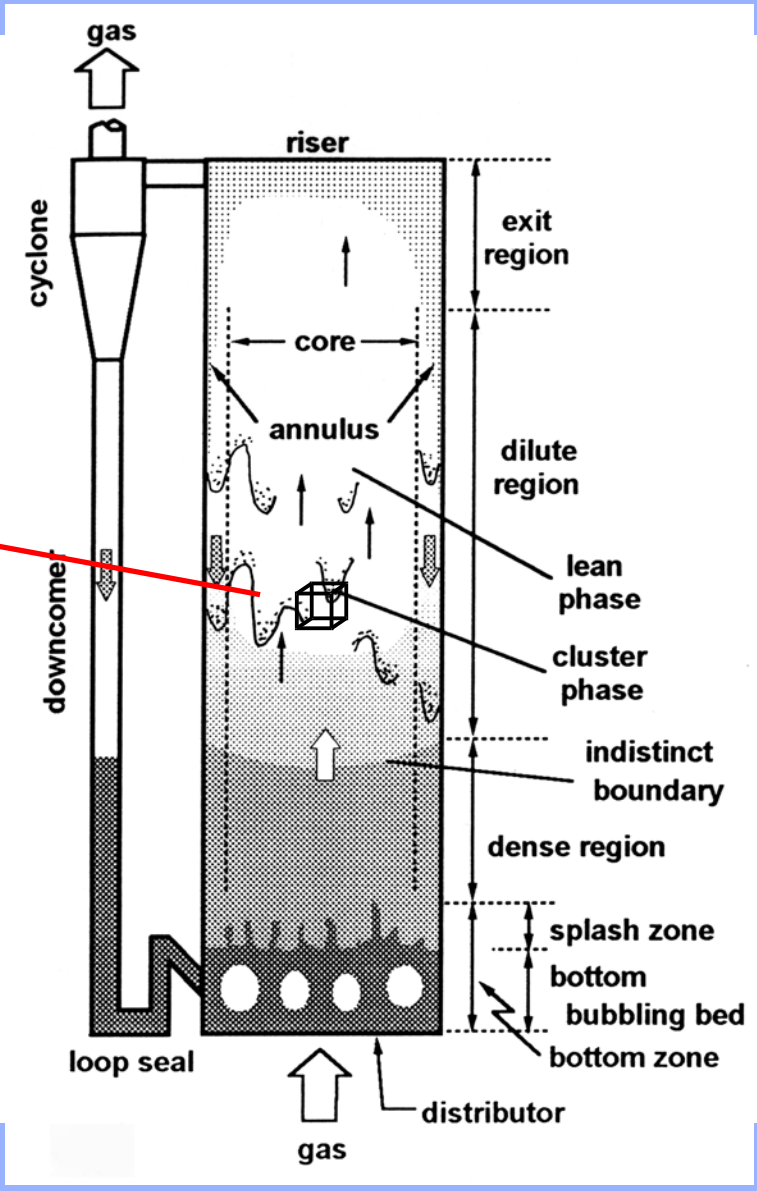
The Traditional Approach

reactor/system	characterizing dimensionless groups
flow tube	$Re,\ Eu,\ L/d$
+ particles in flow tube (two phase flow)	+ $Re_p,\ Fr_p,\ Ar,\ \rho/\rho_p,\ L/d_p,\ \Psi,\ \phi_s$
+ heat transfer to particles	+ $Nu_p,\ Pr$
+ mass transfer to particles	+ $Sh,\ Sc$
+ non-isothermal particles	+ Bi_h
+ concentration profiles in particles	+ Bi_m
+ chemical reactions in flow tube	+ DaI
+ mixing effects	+ $Bo\ (Pe)$
+ chemical reactions inside particles	+ $DaII,\ \phi$

The Concept of Chemical Similarity



Finite Volume



Chemical Similarity Rules - homogeneous systems

A Pure Homogeneous Reaction System:

At a given time, it is:

- gas temperature (T_g)
- total pressure (P)
- species concentration (C_1,...C_i,...C_z)

$$r_{hom,i} = \frac{dN_i}{dt} \cdot \frac{1}{V_R} = f_{hom,i}(T_g, P, C_1, ..., C_i, ...C_z)$$

Chemical Similarity Rules - gas-solid systems

A Gas - Solid Reaction System:

in addition:

- the particle temperature (T_p)
- the gas temperature inside the pores of the particle ($T_{g,pore}$)
- the pressure inside the particle (P_p)
- the species' concentrations inside the pores of the particle ($C_{1,p},...C_{i,p},...C_{z,p}$)
- the species' concentrations at the surface of the particle ($C_{1,s},...C_{i,s},...C_{z,s}$)
- the physical properties of the solid reactant such as external/internal surface area (A_s), pore structure ($X_{p,pores}$)
- the chemical composition of the solid reactant ($X_{p,chem}$)

$$r_{het,i,A} = \frac{dN_i}{dt} \cdot \frac{1}{m_{p,A}} = f_{het,A}(T_{p,A}, T_{g,pore}, P_{p,A}, P, A_{s,A}, X_{p,pores,A}, X_{p,chem,A}, C_{1,p,A},.., C_{i,p,A},.., C_{z,p,A}, C_{1,s,A},.., C_{i,s,A},.., C_{z,s,A})$$

Chemical Similarity Rules - Consequences/Problems

- the actual fuel or solid reactant of the industrial-scale process has to be used in the laboratory-scale
- artificial fuels or solid reactants with well-known compositions can be used as model fuels for the calibration of test units

But even if the same solid reactant is used in laboratory-scale tests different results can be obtained ...

⇒ different heating rates of the solid reactant

⇒ memory effects and fluctuations of conditions

⇒ particle - particle interactions

Chemical Similarity - Conclusions

- It is often not possible to fulfill ***all*** those very stringent similarity rules to derive chemical kinetics in laboratory-scale units.

- However, ***useful information*** can be obtained, if the researcher is ***aware of the problems*** in designing laboratory-scale tests. He or she will know the ***limitations*** and will use the ***obtained results*** in a ***proper way*** depending on the ***aim of the work***.

Thank you for your attention!

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