Succeed at Gas/Liquid Contacting

A wide variety of contactors are available. Here are factors to consider in selection and scale-up.

Operations in which one or more components of a gas phase are absorbed into a liquid phase are common throughout the chemical process industries. In many cases, this contacting serves to achieve desired reactions among components in the two phases.

Three key factors are essential for success of such gas/liquid (G/L) contacting:

1. fluid mechanics, that is, the geometric and physical aspects of the system that govern distribution and flow of the fluids, mixing intensity, and rates of mass and heat transfer;
2. integrity of the equipment, including the impact of corrosion on service life; and
3. kinetics, if a chemical reaction occurs, because it dictates the intrinsically attainable reaction rate.

This article focuses primarily on process considerations, but also addresses interactions with chemical aspects.

Common gas/liquid contactors

Figure 1 depicts nine types of commonly used G/L contactors. Each, of course, has specific attributes that determine its appropriateness for a given service.

Bubble columns

Features:

- low to moderate mixing intensity;
- mixing is caused mainly by the gas, unless liquid is introduced into the column as a jet;
- large liquid holdup;
- long liquid residence time;
- variable extent of backmixing in the liquid phase; and
- gas usually is considered to move in plug flow.

Advantages:

- simple construction, and low capital cost;
- no moving parts, and minimum maintenance;
- ability to handle solids; and
- ease of temperature control.

Disadvantages:

- high pressure drop of the gas due to high static head of the liquid; and
- G/L interfacial area decreases if the ratio of column height to diameter exceeds 12, because of gas bubble coalescence. Staging perforated plates in the column may alleviate the problem, but adds to the pressure drop of the gas and impedes liquid circulation.

Pipes/tubes

Features:

- small diameter, usually < 4 in.;
- horizontal, vertical, and coiled configurations. (In the vertical arrangement, the flow is cocurrent, upwards. For reactions involving evaporating liquid, a vertical configuration can cause "dryout" or "burnout" at the top, and should not be chosen); and
- nearly exclusively operated in a cocurrent mode, suitable for irreversible reactions involving a pure-component gas.

Advantages:

- simple, low-cost construction;
- compactness;
• a wide range of flow rate, pressure, and temperature can be handled; and
• efficient heat exchange.

Disadvantages:
• high pressure drop in both gas and liquid flows; and
• a large number of flow regimes are possible, which may affect contactor performance and complicate the design task.

**Mechanically agitated tanks**

Features:
• impeller type, size, and speed provide additional degrees of freedom to control mixing intensity;
• large liquid holdup;
• broad range of liquid residence times;
• nearly complete liquid back-mixing; and
• considerable gas back-mixing.

Advantages:
• ability to well disperse gas even at low gassing rates;
• can suspend solids; and
• ease of temperature control.

Disadvantages:
• moving parts could incur high maintenance cost; and
• operability at high pressures may be limited by the need to seal the rotating shaft.

**Packed columns**

Features:
• rely on the packing external surface to provide G/L contact;
• 40–60% of the column volume is occupied by the packings;
• packings of less than ⅛-in. dia. can lead to excessive pressure drop; and
• low liquid holdup in the countercurrent mode and in the cocurrent downflow regime.

Advantages:
• low pressure drop of the gas in the countercurrent and trickle-flow regimes;
• corrosion-resistant packings are available for aggressive fluids; and
• can handle foaming liquids in the countercurrent mode and in the cocurrent trickle-flow regime, where little agitation of the liquid by the gas occurs.

Disadvantages:
• G/L flow-rate ratio is restricted by the flooding limit in the countercurrent mode;
• measures must be taken to prevent maldistribution of the liquid; and
• an internal heat exchanger cannot be accommodated readily.

![Figure 1. Common G/L contactors.](image)
Plate/tray columns

Features:
• higher liquid holdup and longer liquid residence time than packed columns;
• large number of transfer units possible;
• nearly complete mixing on each tray;
• overall, behave like continuously stirred-tank reactors (CSTRs) in series;
• countercurrent operation; and
• many types are available, including valve, perforated, bubble-cap, and special proprietary designs. (Valve trays are variable-orifice perforated trays, and, among conventional designs, offer the most flexibility in handling wide ranges of G/L loading. Perforated trays are cheapest; they are ideal if little variation in G/L loading is expected. Bubble-cap trays are more expensive, but less flexible, than valve trays. Proprietary designs can provide higher capacity, but can pose cost and flexibility penalties.)

Advantages:
• can tolerate the presence of solids;
• can accommodate heat-exchanger coils or tubes on trays; and
• offer a wider operating window for gas and liquid flow rates than a countercurrent packed column — that is, they can handle high gas flow rates and low liquid flow rates that would cause flooding in a packed column.

Disadvantages:
• high capital cost, especially when bubble-cap trays or special proprietary designs are used; and
• vulnerable to foaming.

Spray towers

Features:
• liquid is the dispersed phase, gas is the continuous phase; and
• suitable for chemical or physical absorption of highly soluble gases, not suitable for absorption of low solubility gases.

Advantages:
• can handle corrosive fluids and solids-laden gases; and
• ultra-low pressure drop in the gas stream.

Disadvantages:
• high energy consumed for atomizing liquid;
• rapid coalescence of liquid droplets away from the nozzle diminishes mass-transfer efficiency; and
• liquid entrainment in the gas outlet stream.

Jet (loop) reactors

Features:
• can be regarded as a special type of bubble column in which a jet of liquid or G/L mixture is injected into the column at a high velocity;
• mixing in the column is caused entirely by the jet; and
• a draft tube inside the column can be used to effect internal recirculation. An external loop can be created by recycling the liquid.

Advantages:
• higher overall mass-transfer coefficient, \( k_G \), than a conventional bubble column;
• variable degrees of gas self-induction; and
• possible to have 100% utilization of a pure-component gas.

Disadvantages:
• greater power consumption than other alternatives; and
• high attrition of suspending catalysts, if present.

Tubular/venturi ejectors

Features:
• liquid jet is injected into a tube at a very high speed. The tube is of either straight or converging-diverging (venturi) profile. The suction created by the liquid jet aids in gas injection;
• after leaving the injection nozzle, the liquid jet breaks up to become the dispersed phase in a mixing shock zone, and then reverts to the continuous phase further downstream; and
• ultra-high mixing intensity.

Advantages:
• very high mass-transfer coefficient in the mixing shock zone;
• short liquid residence time; and
• small reactor volume.

Disadvantages:
• substantial pumping cost; and
• high attrition of suspending catalysts, if present.

Motionless mixers

Features:
• a pipe with internals; and
• high mixing intensity is brought about by rapid and repeated splitting, twisting, and recombination of the fluids.

Advantages and disadvantages:
• same as those of tubular/venturi ejectors.

Contactor variants

Each contactor type is offered in a variety of configurations, and with numerous possible modifications. For instance, Figure 2 shows various versions of bubble columns (1). Internals such as perforated plates, motionless mixers, or draft tubes can be used to enhance G/L mixing or recirculation in such columns. The recirculation is helpful to prolong residence time, which is favorable for slow reaction, slow mass transfer, or a pure-component gas. On the other hand, recirculation is not advantageous if depletion of the absorbed component occurs in one gas space time, \( \Theta_G \), defined as

\[
\Theta_G = \frac{(V_{GL} \cdot \varepsilon_G)}{Q_G}
\]  

(1)

where \( V_{GL} \) is the volume of the gas and liquid mixture in the reactor, \( \varepsilon_G \) is the gas holdup, and \( Q_G \) is the gas volumetric flow rate.

A bubble column can be configured to operate in a cocurrent downflow mode, but special care must be taken in designing the G/L disengagement compartment to allow stable egress of the gas. It is possible to force 100% utilization of a pure-component gas with the cocurrent downflow operation, though the flow could become unstable outside a narrow window of G/L flow rates, rendering the col-
umn inoperable (2). As indicated in Figure 2, jet (loop) reactors also are called bubble-column reactors by some, especially when the jet is injected into a column and little reaction occurs inside the nozzle.

Packed columns, also known as fixed beds, can be operated countercurrently or in cocurrent downflow or cocurrent upflow, as illustrated in Figure 3 (3). In countercurrent operation, it is impossible to have an upflow liquid stream and downflow gas stream (3). The cocurrent downflow configuration customarily is called trickle bed, though the G/L flow can be outside the trickle-flow regime. The cocurrent upflow configuration also is termed a flooded bed or fixed-bed bubble reactor.

Figure 4 depicts a variety of jet (loop) reactors. Many factors influence design. For instance, will the jet be single- or two-phase, and submerged or plunging? Will one or both fluids be injected? Will a draft tube be provided, and, if so, of what length? And, will there be an internal or external loop? Although the effects of the differences are not well defined, some notable observations have been made.

- For co-injection jets, better dispersion reportedly can be obtained with the gas in the inner tube of a concentric nozzle (4).
- In a plunging liquid-jet reactor, the induction of the gas into the dispersion can be carried out entirely by the jet entrainment action, and 100% utilization of a pure-component gas is feasible.
- The recirculation caused by a draft tube can be investigated by using flow visualization or computational fluid dynamics.

Three commercial jet-loop reactors also are shown in Figure 4. The Buss loop reactor combines a venturi ejector with a bubble column (5,6). It has the feature of a plunging jet reactor with an external loop. The Barbara reactor has special column internals to enhance the internal loop (7,8). The impinging-zone reactor features multiple streams that collide to reintensify the mixing following the initial dispersion in the vicinity of the injection nozzles (9,10).

**Characterizing contactors**

G/L contactors usually are characterized based on the following traits:

- whether operation is continuous or semi-batch;
- the degree of backmixing;
- the relative direction of gas and liquid flows; and
- the attainable mixing intensity as gauged by the mass-transfer coefficient or the G/L interfacial area.

Each of the contactors can run in either: semi-batch or continuous mode. In semi-batch operation, usually there is no net input and output of the liquid, and the gas is charged continuously to the contactor. Truly
batchwise operation, where neither fresh liquid nor fresh gas is fed to the reactor, is rare. Choosing between semi-batch and continuous operation depends upon compatibility with other relevant unit operations, and on considerations related to reactor volume and required residence time.

Complete backmixing is an idealized scenario in which concentration is uniform throughout the reactor. At the other idealized extreme, absolutely no backmixing occurs. It is possible that the gas and liquid phases possess opposite backmixing characteristics.

In the cases where a reaction takes place and is of a positive order, the highest productivity is achieved when backmixing is minimized.

On the other hand, if low concentration of a reactant favors selectivity to the desired product, then complete backmixing is desirable.

A mechanically agitated tank or any other type of reactor with a high liquid recycle ratio is operated in a backmixed mode, and is referred to as a CSTR. A pipe/tube reactor, packed column, plate column, ejector, or motionless mixer normally runs in a nonbackmixed mode and, thus, functions as a plug-flow reactor (PFR). The degree of the backmixing can be represented by a residence time distribution (RTD) curve, and judged by how close it is to that of an ideal CSTR or PFR. More precisely, the reactor can be modeled as a number of CSTRs connected in series. The higher the number of CSTRs required to match the actual RTD curve, the closer the reactor approaches a PFR, and, thus, the lower the backmixing. Alternatively, the degree of backmixing can be quantified by the dispersion coefficient. (Correlation and use of the dispersion coefficient will be discussed later.)

Contactors that possess a certain degree of PFR characteristics can be divided based on the relative direction of the gas and liquid streams. Countercurrent and cocurrent flows are most common, but cross flow is also a possibility. Bubble columns, packed beds, and spray towers can be run in either countercurrent or cocurrent fashion. Pipe/tube and jet loop contactors, ejectors, and motionless mixers usually are operated in cocurrent mode, while tray columns normally function in countercurrent mode. Table 1 provides a general comparison between countercurrent and cocurrent flows.

In cross flow, gas and liquid flow perpendicularly to each other. The content of one phase is progressively added to the flow path of the other phase, resulting in less agitation compared to countercurrent and cocurrent flows, and more uniform concentration of the progressively added phase throughout the contactor. These features can offer significant advantages in some services. For example, less agitation can reduce foaming. Most examples of cross-flow operations are found with liquid-sprayed or gas-sparged contactors in which multiple injections of the dispersed phase are placed along the horizontal path of the continuous phase. Compared to a tall bubble column with either countercurrent or cocurrent flow, the cross-flow option could decrease gas pressure drop, reduce bubble coalescence, and improve the overall mass transfer.

G/L mixing intensity is customarily quantified by a "k_L" or "a" value. The overall mass-transfer coefficient, k_L, is based on the liquid-side concentration differential as the driving force for the mass transfer. The unit of k_L is m/s or equivalent. The G/L interfacial area per unit volume of
the dispersion, \( a \), has the unit of \( m^2/m^3 \) or equivalent. It is much easier to measure the product of \( k_L \) and \( a \) than the individual terms. The value of \( k_L \) depends upon the diffusivity of the dissolved gas in the liquid and the relative velocities between the gas bubbles and the liquid (11). Typically, \( k_L \) varies by at most 100% around a mean value of 0.02 cm/s (12). The value of \( a \) is inversely proportional to the bubble size, and can vary by several orders of magnitude (12). The typical value range of \( k_L a \) or \( a \) is a feature of G/L contactors and the power input. The energy-dissipation rate rises with increasing power input into the contactor, resulting in greater turbulence, which is a major driving force for boosting \( a \). A higher \( k_L a \) can cut capital costs, because the same mixing duty can be achieved in a smaller device, or in a shorter batch time for a batch process or at a higher throughput rate for a continuous process.

Another measure of mixing intensity is gas holdup, \( \varepsilon_g \). It is defined as the ratio of the volume of the gas in the mixture to the total volume of the mixture. Table 2 compares common G/L contactors on the typical value range of \( k_L a \), \( \varepsilon_g \), \( V_p \) (contactor volume), \( \varepsilon_L \) (power dissipation per unit volume), and the backmixing property of the gas and liquid flows (13). Table 3 contrasts three types of packed columns, suggesting that the cocurrent upflow mode is more power efficient than the cocurrent downflow mode in the pulse and spray flow regimes. Table 4 compares various types of jet
(loop) reactors. The $k_a$ values listed in the tables are for the $O_2$ (air)/water pair measured from physical absorption or desorption. Care must be exercised when comparing $k_a$ values reported in the literature, however. In a chemical method, e.g., sulfate oxidation, the sulfate solution inhibits bubble coalescence, and there is mass-transfer enhancement due to the reaction. Therefore, $k_a$ measurements via a chemical method will be higher than those from a physical method. It has been reported that in a mechanically agitated tank under the same operational conditions, $k_a$ measured from the chemical method is about seven times as high as that measured from the physical method (14).

### Choosing a contactor

#### Wish list

An approach to select a suitable G/L contactor is to compose a wish list. Then, narrow the choices by ruling in or out contactors based on the features, advantages, and disadvantages of each contactor. Finally, perform an economic analysis to determine the final selection.

Consider factors such as the following for your wish list:
- maximum conversion of reactants;
- greatest selectivity for desired products;
- safety, such as reliable temperature control, least holdup of hazardous materials, and so on;
- minimum environmental impacts;
- excellent ability to accommodate variation in operational conditions or capacity requirements;
- ease of automation and process control;
- simplicity of scale-up; and
- low capital and operating costs.

Here are some examples of how to rule in or rule out contactors:
- If moving parts are not allowed, rule out the mechanically stirred tank and the spray device.
- If particles are contained in the liquid feed or formed during the reaction, rule out the packed column.
- To minimize foaming, rule in the packed column with countercurrent flow and spray tower, rule out the jet loop reactor, the ejector, and the motionless mixer.

### Table 1. How countercurrent and cocurrent flows generally compare.

<table>
<thead>
<tr>
<th>Countercurrent</th>
<th>Cocurrent</th>
</tr>
</thead>
<tbody>
<tr>
<td>Better when the component to be absorbed constitutes a small fraction of the gas</td>
<td>Better when the gas is composed of only one component</td>
</tr>
<tr>
<td>Suitable for physical absorption and reversible reactions</td>
<td>Suitable for irreversible reactions</td>
</tr>
<tr>
<td>Driving force for mass transfer is more uniform regardless of the number of components in the gas</td>
<td>Driving force decreases in the flow direction if the gas contains more than one component, or is constant in the case of a pure-component gas</td>
</tr>
</tbody>
</table>

### Table 2. Attributes of common G/L contactors.

<table>
<thead>
<tr>
<th>Contactor</th>
<th>$k_a$</th>
<th>$a_0$</th>
<th>$e_0$</th>
<th>$V_r$</th>
<th>$e_p$</th>
<th>Backmixing</th>
<th>Liquid Flow</th>
<th>Backmixing</th>
<th>Gas Flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble column excluding jet (loop)</td>
<td>0.025–0.06</td>
<td>-20</td>
<td>&lt;0.2</td>
<td>0.022–300</td>
<td>0.01–1</td>
<td>CSTR–PFR</td>
<td>CSTR–PFR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spray column</td>
<td>0.007–0.01</td>
<td>10–100</td>
<td>&gt;0.8</td>
<td>—</td>
<td>—</td>
<td>CSTR</td>
<td>CSTR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Packed column, countercurrent</td>
<td>0.005–0.02</td>
<td>-200</td>
<td>&gt;0.95</td>
<td>0.005–300</td>
<td>0.01–0.2</td>
<td>PFR</td>
<td>PFR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Plate column</td>
<td>0.01–0.05</td>
<td>100–400</td>
<td>&gt;0.8</td>
<td>0.005–300</td>
<td>0.01–0.2</td>
<td>CSTR–PFR</td>
<td>CSTR–PFR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pipe/tube</td>
<td>0.01–0.7</td>
<td>50–2,000</td>
<td>0.05–0.95</td>
<td>—</td>
<td>0.1–10</td>
<td>PFR</td>
<td>PFR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mechanically agitated tank</td>
<td>0.02–0.2</td>
<td>-200</td>
<td>&lt;0.1</td>
<td>0.002–100</td>
<td>0.5–4</td>
<td>CSTR</td>
<td>Intermediate–PFR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Jet (loop)</td>
<td>0.01–0.2</td>
<td>200–2,000</td>
<td>&lt;0.5</td>
<td>0.02–100</td>
<td>0.8–90</td>
<td>CSTR–Intermediate</td>
<td>CSTR–Intermediate</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tubular/venturi ejector and motionless mixer</td>
<td>0.1–3</td>
<td>1,000–7,000</td>
<td>&lt;0.5</td>
<td>&lt;10</td>
<td>10–700</td>
<td>PFR</td>
<td>PFR</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Modified from Ref. 13.

* Typical for $O_2$ (air)/water unless noted otherwise.

*† For typical pipes/tubes of diameter on the order of an inch. For the monolith of diameter on the order of mm, $k_a$ can be as high as $3 \times 1$, and $e_p$ as high as $1,000 \text{ kW/m}^2$.

† Taken from Ref. 16, including values for G/L pairs other than $O_2$/water.

†† Calculated as the ratio of the gas-flow rate to the sum of the gas and liquid flow rates, which may not be a valid assumption.

† Because a spray column is considered to have only one or, at most, two equilibrium stages (16,23).

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Table 3. Impact of different flow directions on packed columns

<table>
<thead>
<tr>
<th>Flow Direction</th>
<th>Flow Regime</th>
<th>Liquid Holdup</th>
<th>$e_p$ kW/m²</th>
<th>Solid Wetting</th>
<th>Axial Dispersion</th>
<th>Pressure Drop</th>
</tr>
</thead>
<tbody>
<tr>
<td>Countercurrent</td>
<td>Liquid Rivulets</td>
<td>0.005–0.01</td>
<td>&lt;0.05</td>
<td>0.01–0.2</td>
<td>Lower</td>
<td>Lower</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Low</td>
<td></td>
</tr>
<tr>
<td>Co-current,</td>
<td>Downflow</td>
<td>Trickle</td>
<td>0.005–0.01</td>
<td>0.01–0.2</td>
<td>Low</td>
<td>Low</td>
</tr>
<tr>
<td></td>
<td>Pulse and spray</td>
<td>0.1–0.2</td>
<td>0.1–0.9</td>
<td>0.05–15</td>
<td>*</td>
<td>Higher</td>
</tr>
<tr>
<td>Co-current,</td>
<td>Upflow</td>
<td>Bubble</td>
<td>0.005–0.01</td>
<td>0.01–0.2</td>
<td>High</td>
<td>High</td>
</tr>
<tr>
<td></td>
<td>Pulse and spray</td>
<td>20–80%</td>
<td>0.1–0.9</td>
<td>0.02–5</td>
<td>*</td>
<td>Higher</td>
</tr>
</tbody>
</table>

* In pulse flow, solid wetting is high in the liquid-rich block and low in the gas-rich block. In spray flow, the solid wetting is low at any instant, but the solid is bombardeed frequently by liquid droplets.
† No data available.

- To accommodate internal coils/tubes or a wall jacket for heat exchange, rule in the bubble column, the mechanically stirred tank, the pipe/tube reactor, and the plate column; rule out all others.

- To minimize the liquid inventory in the contactor, rule in the countercurrent packed column, the trickle bed, and the plate column; rule out the bubble column, the mechanically stirred tank, and the jet loop reactor. The ejector and the motionless mixer might be applicable, because their volume is usually smaller and the total liquid holdup may be acceptable.

Selection based on mixing intensity

If only physical absorption or desorption is contemplated, selection of a proper $k_{la}$ value is a simple matter of assessing the tradeoff between the capital and operating costs. When a reaction is involved, the proper $k_{la}$ value depends upon the intrinsic reaction kinetics. If the desired reaction is slow, a high $k_{la}$ may not offer any advantage. On the other hand, in a fast reactor where mass transfer becomes the rate-limiting step, a high $k_{la}$ should improve the conversion and possibly also the selectivity.

The Hatta number provides a basis for assessing the relative rates of mass transfer and reaction. In most cases, the reaction between the dissolved gas (A) and a component (B) in the liquid is irreversible and first order with respect to each component; its intrinsic reaction rate, $r$, can be represented as:

$$ r = k \cdot c_{AL} \cdot c_{BL} $$ (2)

where $k$ is the reaction rate constant, $c_{AL}$ and $c_{BL}$ are the concentrations of A and B, respectively, in the liquid bulk. The Hatta number is defined as

$$ Ha = \sqrt{\frac{D_{AL}}{k \cdot c_{BL}}} $$ (3)

where $D_{AL}$ is the diffusivity of the dissolved gas in the liquid.

If $Ha < 3$, the net reaction rate is not limited by the mass transfer (more details can be found in Ref. 15). Note that evaluation of $Ha$ requires considerable knowledge about the G/L system in question. In addition to $k$ and $D_{AL}$, $c_{BL}$ can be determined from the feed concentration and the targeted conversion, $k_l$ has to be computed from $k_{la}$ and $a$. If the reaction is not first order with respect to the dissolved gas, $Ha$ is a function of $c_{AL}$, which cannot be estimated $a priori$ in most cases — the evaluation of $Ha$ becomes impossible.

Bear in mind that while a sufficiently high $k_{la}$ value is desirable, so as not to limit the intrinsic reaction rate, it may not be economic. Furthermore, the conversion of the key reactant may not be linearly proportional to $k_{la}$; thus, the return from increasing $k_{la}$ may diminish beyond a certain level. Proper choice of $k_{la}$, as well as other operational variables, can be accomplished through mathematical modeling, if the reaction kinetics are known.

The significance of liquid bulk

In addition to the overall mass-transfer rate, the magnitude of gas (or liquid) holdup also can be an important consideration depending upon the objective of the G/L contacting. If the goal is liquid processing, for instance, converting a component in the liquid phase or simply impregnating the liquid with the dissolved gas, a contactor offering a high liquid holdup is desired. On the other hand, if the objective is gas conditioning, such as removal of CO₂ from wellhead natural gas, a contactor providing a high gas holdup is preferred.

To combine the liquid holdup with constants related to the mass transfer, a dimensionless parameter, $\beta$, is defined:

$$ \beta = \frac{\varepsilon_L}{a \cdot \delta} $$ (4)

where $\varepsilon_L$ is the liquid holdup, and $\delta$ is
the thickness of the liquid-side diffusion film. $\beta$ represents the ratio of the liquid-phase volume in the contactor to the volume of the diffusion film. Note that $\delta$ is obtained as the ratio of the diffusivity to the liquid-side mass-transfer coefficient, that is:

$$
\delta = \frac{D_{\text{A}}}{k_{\text{L}}} = \frac{D_{\text{A}}}{k_{\text{L}}}
$$

Typical $\beta$ values for selected contactors are given in Table 5 (12,16).

For slow reactions, Krishna suggests choosing a high $\beta$ contactor, because most of the reaction occurs in the liquid bulk. For fast reactions in which most of the reaction takes place in the diffusion film, the liquid bulk makes little contribution; so, low $\beta$ contactors should be used (16). Most gas-conditioning operations involve chemisorption with fast reaction; this consideration and the capacity criterion both point to a low $\beta$ contactor.

If the reaction heat has to be managed through the liquid bulk, a contactor of moderate or high $\beta$ may still be the right choice in spite of a fast reaction.

**Selectivity considerations**

The selectivity for a desired product made in the liquid phase can be best illustrated by considering two classical examples: consecutive and parallel reactions (12,17-19).

**Consecutive reactions.**

$$
A_{(g)} + B_{(l)} \rightarrow D_{(l)} \quad \text{Desired product}
$$

$$
D_{(l)} + A_{(g)} \rightarrow U_{(l)} \quad \text{Undesired byproduct}
$$

where (g) and (l) denote gas and liquid phases. The chlorination of hydrocarbons is an example of this type of reaction. The selectivity of the desired product, $D$, is favored by the following conditions that serve to "short" the undesired subsequent reaction: high $\beta$; low $k_{lA}$: PFR characteristic; staged injection of $A$ (cross flow); and short liquid residence time. These conclusions are independent of the ratio of the reaction rate constants and the ratio of the reaction orders. The sensitivity is more conspicuous if the desired reaction is the faster one.

The conditions of high $\beta$, low $k_{lA}$, and short liquid residence time, however, adversely affect the reaction conversion. Because the yield of $D$ is proportional to the product of the conversion and the selectivity, optimum values of $\beta$, $k_{lA}$, and liquid residence time must be sought to maximize the yield.

**Parallel reactions.**

$$
A_{(g)} + B_{(l)} \rightarrow D_{(l)}
$$

with a reaction rate

$$
r_1 = k_1 \cdot c_{A}^{m} \cdot c_{B}^{n}
$$

$$
A_{(g)} + C_{(l)} \rightarrow U_{(l)}
$$

with a reaction rate

$$
r_2 = k_2 \cdot c_{A}^{m} \cdot c_{C}^{n}
$$

In this reaction class, B and C could be the same component. The oxidation of cyclohexane to cyclohexanone and cyclohexanol is an example of this type of reaction. Depending upon the relative magnitudes of the reaction orders, the effects of the reactor type and operating conditions on the selectivity of $D$ differ.

1. $m = n$

The selectivity only depends upon the intrinsic kinetics, that is, $k_1/k_2$. Reactor type and operating conditions have no effect.

2. $m > n$

The selectivity improves with increasing concentration of the dissolved gas. Hence, high $k_{lA}$ and PFR characteristics are favorable. The sensitivity is more noticeable with a greater $k_{lA}/k_{lC}$ ratio.

3. $m < n$

The selectivity is favored by a low concentration of the dissolved gas. Thus, low $k_{lA}$, CSTR characteristics, and staged injection of the gas (cross flow) are desired. The sensitivity is more obvious with a smaller $k_{lA}/k_{lC}$ ratio. In this case, the gas will be wasted on the undesired reaction or due to low absorption efficiency. If the gas is expensive, and B and C are different components, then it may be worthwhile to remove C prior to the reaction step or use a catalyst to alter the chemistry, etc.

Like conversion, selectivity is amenable to analysis by mathematical modeling, if values of the kinetics constants and relevant parameters are known.

---

**Table 4. Performance of various jet (loop) reactors with G/L co-injection.**

<table>
<thead>
<tr>
<th>Type</th>
<th>$k_{B,L}$ 1/s</th>
<th>$c_{B}$ kW/m²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Downflow, no draft tube</td>
<td>0.04-0.08</td>
<td>0.8-2.5</td>
</tr>
<tr>
<td>Downflow, with draft tube</td>
<td>0.01-0.1</td>
<td>1-5</td>
</tr>
<tr>
<td>Burdoss loop reactor, upflow</td>
<td>0.1-2.2</td>
<td>8-90</td>
</tr>
</tbody>
</table>

* For O₂ (air)/water.

**Table 5. Typical values of $\beta$ for various G/L contactors.**

<table>
<thead>
<tr>
<th>Contactor</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble column</td>
<td>10⁻¹⁰⁻³¹</td>
</tr>
<tr>
<td>Mechanically agitated tank</td>
<td>10⁻¹⁰⁻³¹</td>
</tr>
<tr>
<td>Trickle bed and countercurrent packed bed</td>
<td>10⁻¹⁰⁻³¹</td>
</tr>
<tr>
<td>Plate column in spray regime</td>
<td>10⁻¹⁰⁻³¹</td>
</tr>
<tr>
<td>Ejector</td>
<td>10⁻¹⁰⁻³¹</td>
</tr>
<tr>
<td>Spray tower</td>
<td>10⁻¹⁰⁻³¹</td>
</tr>
</tbody>
</table>
An example. For gas processing, contactor choices should be limited to those providing high gas holdup. In this example, \( \text{H}_2\text{S} \) is to be selectively absorbed from a gas stream containing \( \text{CO}_2 \) by amine solutions (16). The reaction of \( \text{H}_2\text{S} \) with the amine is faster than that of \( \text{CO}_2 \). More importantly, \( \text{H}_2\text{S} \) has higher solubility than \( \text{CO}_2 \), so that the overall mass transfer of \( \text{H}_2\text{S} \) is limited by the gas-side resistance, whereas the liquid-side resistance dominates for \( \text{CO}_2 \). Therefore, increasing the gas-side turbulence should enhance the \( \text{H}_2\text{S} \) mass transfer with little influence for \( \text{CO}_2 \). By doubling the gas velocity in a tray column, the G/L contacting pattern is shifted from the froth to the spray regime, and the \( \text{H}_2\text{S} \) selectivity is nearly doubled.

**Flow aspects**

**Flow regimes**

Flow condition critically influences mass and heat transfer, and determines mixing quality. When scaling up a G/L reactor, it is important to maintain the same flow regime.

**Bubble columns.** Three flow regimes have been observed in bubble columns: bubbly flow, churn-turbulent flow, and slug flow. At low gas superficial velocities, bubbles are quite uniform in size at the same height in the column; they rise in orderly fashion with little collision among bubbles. This is bubbly flow, also dubbed homogeneous or quiescent flow, in which the liquid is mildly stirred by the bubbles. When the gas velocity is higher than about 5 cm/s, bubbles of different sizes can be found at the same height in the column, due to increased coalescence; they churn up the liquid, significantly increasing the mixing intensity. This is churn-turbulent or heterogeneous flow, in which circulation of the liquid and, to a lesser extent, gas is noticeable. In a column of diameter less than about 15 cm at high gas velocities, bubbles are predominantly in the form of slugs whose cross-section almost spans the entire column diameter. This is called slug flow.

Figure 5 includes schematics of the three flow regimes and a chart showing the transition (1,20). The flow regime depends primarily upon the gas superficial velocity. The column diameter also can be influential if it is less than 15 cm. The gas velocity for the transition between the bubbly and churn-turbulent flows increases with increasing pressure, and with the use of a porous-plate gas sparger (1). With a highly viscous liquid, slug flow dominates (21).

**Mechanically agitated tanks.** Bubbly distribution and flow pattern are the major characteristics and concerns of the flow regime in a mechanically stirred tank. The condition changes mainly with the impeller speed, \( N \), and gas-flow rate, \( Q_G \). Figure 6a depicts various bubble flow patterns (13). The flow pattern affects the power drawn into the G/L mixture; the power draw, in turn, determines the mass-transfer coefficient and gas holdup (as will be discussed later). The dependence of the power draw on the flow pattern is demonstrated in Figure 6b for Rushton turbines (13). For a constant \( Q_G \) at lowest \( N \) (regions a and b in Figure 6a), the gas passes mostly through the impeller without dispersion and the liquid flows around the outer part of the blades undisturbed by the gas. The impeller is said to be flooded. In this flow regime, the gassed power draw, \( P_{G*} \), is close to the ungassed power draw, \( P_{U*} \), at the same \( N \). As \( N \) increases to \( N_T \), the gas is captured by the vortices behind the impeller blades and the im-
peller is said to be loaded. The gas becomes dispersed across the tank cross-section, and \( P_G \) begins to decrease as the captured gas forms large cavities behind the blades. Further increase of \( N \) diminishes the gas cavities and changes their form. The \( P_G/P_U \) curve passes through a minimum at an impeller speed \( N_{CD} \), which is the minimum speed to just completely disperse the gas throughout the whole tank. Increasing \( N \) further, small recirculation patterns start to emerge, region d in Figure 6a, and the power draw curve begins to rise from the minimum. The maximum point on the power draw curve corresponds to the impeller speed, \( N_{R} \), at which gross recirculation of the gas back into the agitator starts. Each flow pattern sees a particular form of gas cavities behind the agitator blades (22). The flow regime in which the impeller is flooded should be avoided.

Correlation equations for \( N_F \), \( N_{CD} \), and \( N_R \) have been developed for the standard 6-blade Rushton turbine (12):

\[
\frac{Q_G}{N_{i} \cdot d_i^2} = 30 \left( \frac{d_i}{d_T} \right)^{3.5} \left( \frac{N_{FP} \cdot d_i}{g} \right)
\]

(6)

\[
\frac{Q_G}{N_{CD} \cdot d_i^2} = 0.2 \left( \frac{d_i}{d_T} \right)^{0.5} \left( \frac{N_{CDP} \cdot d_i}{g} \right)^{0.5}
\]

(7)

\[
\frac{Q_G}{N_{F} \cdot d_i^2} = 13 \left( \frac{d_i}{d_T} \right)^5 \left( \frac{N_{FP} \cdot d_i}{g} \right)^2
\]

(8)

Flow regime maps for other impellers can be found in Ref. 13. For special impellers, consult vendors about flow regimes and the correlation with \( N \), \( Q_G \), and relevant geometric dimensions.

Pipes/tubes. Flow patterns and maps are shown in Figure 7 for horizontal pipes and Figure 8 for vertical pipes (23). Slug flow should be avoided, because it causes severe vibration of the pipe due to the impact of slugs on pipe beads and other fittings. Spray (or mist) and annular patterns generate the largest interfacial area and cause rapid interface renewal. They are preferable when high \( k_{i,d} \) is desired. Bubble flow could be satisfactory even in horizontal pipes in which the bubbles are confined to the top of the pipe, provided that mass transfer is sufficiently rapid compared to reaction rate. When relatively large amounts of gas are absorbed, the flow pattern can change along the length of the reactor and the danger of passing to undesired flow regimes must be considered. Figures 7 and 8 are helpful for this purpose.

Packed columns — countercurrent. Countercurrent flow in a packed column is characterized by the percentage of flooding, which is the operating gas velocity as a percentage of the flooding velocity. For given gas and liquid mass-flow rates, column diameter must be chosen so that the flooding falls between 30% and 70%. Figure 9 is a generalized chart for
flooding and pressure drop (24). To use Figure 9,

1. Calculate the x-axis value from the given gas and liquid mass-flow rates and densities.

2. At the calculated x-axis value, locate the point on the flooding line. Read out its y-axis value.

3. From the y-axis value, back out the corresponding gas flux, \( G \). This is the flooding gas mass flux.

4. Multiply the flooding gas flux by a flooding percentage, for instance, 50\% (a value chosen by considering the gas pressure drop, see Step 6 below). This is the operating gas flux.

5. From the operating gas flux and the given gas-flow rate, calculate the column diameter.

6. Calculate the y-axis value corresponding to the operating gas flux. From the calculated y-axis value and the previously calculated x-axis value, determine the curve in Figure 9 passing through the intersection point. The parameter value for this curve is the pressure drop of the gas flow, in. water/ft packed height. If the pressure drop is not satisfactory, go back to Step 4 and use a modified flooding percentage.

**Packed columns — cocurrent, downflow.** Figure 10 depicts the flow maps for cocurrent downflow in a packed column (25). With nonfoaming liquids, trickle, pulsed, and spray flows are possible. With foaming liquids, spray flow has not been reported; instead, trickle, foaming, foaming pulsed, and pulsed flow have been observed. In trickle flow, the gas is the continuous phase; the liquid trickles over the packings in the discontinuous shape of films, rivulets, and drops. In this regime, the liquid flow is laminar, while the gas flow is laminar or turbulent. As its flow rate increases, the gas exerts more drag on the liquid, causing some liquid to separate from the liquid film and move as slugs or drops down a channel before reforming over the packings. The separated slugs and drops grow and become large enough to bridge channels. This momentary blocking of some channels causes the liquid to accumulate, leading to the development of liquid-rich and gas-rich regions pulsing down the column. As the gas flow increases further, the liquid-continuous blocks are blown apart; the liquid becomes a heavy mist carried down the column in the gas stream. This is called spray flow. The trickle flow is referred to as a “poor interaction” regime, because of the relatively stagnant situation. The other flow regimes are denoted as “high interaction.” At a constant flow rate of a foaming liquid, foams may develop due to surface rippling of the liquid film and rivulets in the mid-range of gas-flow rates.
Packed columns — cocurrent, upflow. At low gas-flow rates, bubbly flow occurs. As shown in Figure 11 (25), there is inconsistency in the literature about the transition to slug and spray flow regimes as the gas-flow rate increases. The slug flow is similar to pulsed flow in a trickle bed. Shah (25) recommends use of Figure 11b for an air/water system.

Tray columns. Froth flow changes to spray flow as the gas-flow rate increases. The liquid is the continuous phase on a tray in the froth regime, and the dispersed phase in the spray regime. The percentage flooding also is used to characterize the flow condition; see pp. 14-28 of Ref. 24a for more details.

Tubular/venturi ejectors. In a tubular or venturi ejector, liquid is injected at a high velocity. The liquid jet is broken down by the gas flow and becomes the dispersed phase in the mixing shock zone. Further downstream, the liquid becomes the continuous phase and the gas breaks into bubbles. This regime is called bubbly flow. Figure 12 illustrates the flow transition and the dependence on the relative volumetric flow rates (26). The flow map of Figure 12c is valid only for that particular ejector. The figure probably would be applicable regardless of nozzle and ejector sizes if the x-axis was the liquid jet velocity. A swirl component of the liquid jet velocity would shorten jet flow and mixing shock zone, as shown in Figures 12d and 12e. It also would increase gas suction and lower k_{ga} (27).

Pressure drop
To estimate gas absorption, reaction conversion, or product yield, it usually suffices to assume constant gas pressure, especially in a reactor exhibiting CSTR characteristics. If the gas stream has a certain degree of PFR characteristics, the estimation can be improved by considering the variation of the gas pressure along the flow path. Pressure drops in the gas and liquid streams are needed, however, for sizing a pump, blower, or compressor.

For the liquid stream, the pressure drop is due mainly to the elevation. When a liquid nozzle or a G/L co-injection nozzle is used, as in spray towers, jet loop reactors, and ejectors, the velocity head at the nozzle could be the major component for the pressure drop. In pipe/tube reactors, friction drag cannot be neglected. For cocurrent, upflow in a packed column, the packing contributes signifi-
cantly to the pressure drop because of the friction or form drag. In motionless mixers, both the friction and form drags are the main causes for pressure drop.

When the gas is the dispersed phase and in the upflow direction, pressure drop is due mainly to the total height of the ungassed liquid. In tray columns, the additional pressure drop due to orifices or bubble caps must be included. The pressure drop in spray towers, but not in associated pipes and pipe fittings, is negligible. In packed columns, countercurrent or trickle flow, the pressure drop is minimal, but not negligible. (We already have explained how to calculate the pressure drop in countercurrent packed columns.) The comments in the previous paragraph about the liquid-flow pressure drop in pipe/tube reactors, cocurrent upflow in packed columns, and motionless mixers also apply to gas flow.

For details on calculating pressure drop in various reactors, see the following sources:

Pipe/tube reactors, p. 662 of Ref. 23, pp. 6-26 of Ref. 24a;

Packed columns — countercurrent, pp. 14-42 of Ref. 24a, and p. 276 of Ref. 25 (as well as earlier in this article);

Packed columns — cocurrent, downflow, p. 184 of Ref. 25;

Packed columns — cocurrent, upflow, p. 232 of Ref. 25; and


**Transport coefficients**

Transport coefficients are important building blocks of the dynamic similarity principle for scaling up reactors. Impacts of primary design and operational variables on reactor performance can be best explained and controlled through understanding of transport coefficients. The effects of the transport coefficients on reactor performance will be addressed later.

For most $G/L$ systems of practical interest, gas solubility is low. Thus, the overall mass-transfer coefficient is limited by the liquid-side resistance and is represented by $k_L a$.

Gas or liquid holdup could be influential for continuous processes. For batch or semi-batch processes, the holdup is needed for estimating the expansion of the liquid when gassed, which is important when considering a capacity increase for an existing vessel. Gas and liquid dispersion coefficients indicate the degree of deviation from plug-flow characteristics, a concern only for bubble columns and packed beds. Finally, the heat-transfer coefficient is an important factor for reaction heat management.

**Bubble columns**

**Mass-transfer coefficient, $k_L a$**

For aqueous and alcohol liquids, Eq. 9 developed by Hikita et al. (28) is recommended. In it, $k_H$

$$= 1$$

for non-electrolytes, $= 10^{0.087/2}$ for liquid containing electrolytes with an ionic strength, $I$, $<1$ kg ion/m$^3$, or

$$= 1.14 \times 10^{0.021}$$

for liquid containing electrolytes with $I >1$ kg ion/m$^3$.

For organic liquids other than alcohols, use Eq. 10, which was developed by Ozturk and coworkers (21), in which $d_p$ can be assumed to be approximately 0.003 m.

For non-Newtonian liquids, if the power law applies and elasticity can be quantified by the first normal stress difference, then the following equation developed by Suh et al. (21) is recommended:

$$Sh' = 0.018 \times Sc^{0.5} \times Bo^{0.2} \times Ga^{0.62}$$

$$\times F_r^{0.51} \times (1 + 0.12 W_f)^{-1} \quad (10)$$

where

$$Sh' = \text{Sherwood Number}$$

$$= (k_L a d_p^2)/D_L$$

(11)
and $k_l a'$ is based on liquid volume instead of $G/L$ mixture volume.

$$
S_c = \text{Schmidt Number} = \mu_{L_{eff}}/(\rho_l \cdot D_L) \tag{13}
$$

$B_o = \text{Bond Number}$

$$
G_a = \text{Galilei Number} = (g \cdot d_i^3 \cdot \rho_l^2 \gamma) / \mu_{L_{eff}} \tag{15}
$$

$F_r = \text{Froude Number} = u_G/(g \cdot d_i)^{0.5} \tag{16}$

**Equation 9.**

$$
k_{lG} \cdot u_G = 14.9 \cdot k_H \left( \frac{u_G \cdot \mu_l}{\sigma} \right)^{1.76} \left( \frac{\mu_l \cdot g}{\rho_l \cdot \sigma^3} \right)^{0.248} \left( \frac{\mu_l}{\mu_l} \right)^{0.243} \left( \frac{\mu_l}{\rho_L \cdot D_l} \right)^{-0.604} \tag{17}
$$

**Equation 10.**

$$
k_{lG} \cdot d_i^2 / D_L = 0.62 \left( \frac{\mu_l}{\rho_L \cdot D_L} \right)^{0.5} \left( \frac{g \cdot \rho_l \cdot d_i^3}{\sigma} \right)^{0.33} \left( \frac{g \cdot \rho_l^2 \cdot d_i^3}{\mu_l^3} \right)^{0.29} \left( \frac{u_G}{\sqrt{g \cdot d_i}} \right)^{0.65} \left( \frac{\rho_G}{\rho_L} \right)^{0.04} \tag{18}
$$

$Wi = \text{Weissenberg Number} = N_l / \tau_{eff} \tag{19}$

where $N_l = \text{first normal stress difference}$,

$\tau_{eff} = \text{effective shear stress} = \mu_{L_{eff}} \cdot \dot{\gamma}_{eff} \tag{20}$

$\dot{\gamma}_{eff} = \text{effective shear rate} = 2,800 \cdot u_G$, with $u_G$ in m/s.

Bear in mind several points:

1. $k_{lG}$ (and $\varepsilon_G$) is independent of column diameter, $d_c$, provided $d_c \geq 0.15$ m (1,21).

2. $k_{lG}$ is not affected by gas sparger type if $u_G > 0.03$ m/s. At lower gas velocities, sintered plate spargers give rise to higher $k_{lG}$ than single-hole or perforated spargers (29).

3. The effect of solids on $k_{lG}$ depends upon gas velocity, liquid velocity (for continuous process), solid particle size and concentration, etc. For the typical operating conditions prevailing in Fisher-Tropsch synthesis (particle diameter < 50 µm, solid concentration < 16 wt. %), the solid has negligible effect on $k_{lG}$ (1).

4. Reports in the literature about the effect of pressure on $k_{lG}$ are not consistent (29).

5. References 1, 21, and 29 list more correlations, but do not give conclusive recommendations. Reference 29 lists several correlations for $k_L$.

Gas holdup, $\varepsilon_G$. Hikita and coworkers developed Eq. 21 (30) where $k_H$

$$
k_H = 1$ for nonelectrolytes,

$= 10^{0.044 \cdot l}$ for liquid containing electrolytes with $l \leq 1$ kg ion/m³, or

$= 1.1$ for liquid containing electrolytes with $l > 1$ kg ion/m³.
In the quiescent (bubbly) flow regime, \( \varepsilon_g \) can be approximated as 
\[ \varepsilon_g = 4 \, \mu \frac{u_g}{u_G} \text{ if } u_g < 0.05 \text{ m/s} \]
(21)
For non-Newtonian liquids, the following equation developed by Deckwer and Schumpe (21) is recommended:
\[ \varepsilon_g = 0.2 \, B \alpha^{0.13} \, \Gamma d_{L}^{0.11} \, \eta^{-0.54} \]
(23)
where the dimensionless groups are defined as in Eqs. 14–16.

References 1 and 21 give more correlations.

Bubble diameter, \( d_b \). In the quiescent and churn-turbulent flow regimes, the prevailing bubbles range from \( \frac{1}{16} \) in. to \( \frac{3}{8} \) in. (31). Using single-orifice, perforated-plate, and sintered-plate gas spargers, Akita and Yoshida developed Eq. 24 (32).

To apply this equation for columns of diameter greater than 0.3 m, use \( d_{C} = 0.3 \) m in the calculation.

Liquid dispersion coefficient, \( E_L \). This depends upon gas velocity and column diameter. The influence of liquid properties is not clearly understood (1). Combining the work of several investigators, Deckwer and Schumpe (21) recommended the following equation:

\[ E_L = 0.35 \left( \frac{g \cdot d_{C}^{5}}{u_{G}^{3}} \right)^{0.33} \]
(25)

Another, more complex equation developed by Joshi and Sharma can be found in Reference 1.

There is a rule of thumb to assess the mixing in the liquid phase. Define

\[ \Phi = \frac{H^2 \cdot k_l \alpha}{E_L \cdot \bar{E}_L} \]
(26)
in which \( H \) is the column height. If \( \Phi \ll 1 \), the concentration of absorbed gas is uniform in the liquid throughout the column (21).

Gas dispersion coefficient, \( E_G \). Reported \( E_G \) data are inconsistent. Nevertheless, the following equation of Wachi and Nojima (21) may be used:

\[ E_G = 20 \, d_c^{5} \cdot u_G \]
(27)
with \( E_G \) in m/s, \( d_c \) in m, and \( u_G \) in m/s.

**Equation 21.**

\[ \varepsilon_g = 0.672 \, k_{H} \left( \frac{u_G}{u} \right)^{0.578} \left( \frac{\mu_g}{\mu} \right)^{0.013} \left( \frac{\rho_g}{\rho_L} \right)^{0.062} \left( \frac{\mu_g}{\mu_L} \right)^{0.107} \]

**Equation 24.**

\[ \frac{d_h}{d_c} = 26 \left( \frac{d_c \cdot g \cdot \rho_L}{\rho} \right)^{0.5} \left( \frac{g \cdot d_c^{5} \cdot \rho_L}{\mu_L} \right)^{0.12} \left( \frac{u_G}{\sqrt{g \cdot d_c}} \right)^{0.12} \]
Assuming CSTR behavior for the gas phase is justified only if the gas Bodenstein number is greater than 10 (21), that is

$$Bd = \frac{u_G \cdot H}{e_G \cdot E_G} \geq 10 \quad (28)$$

An important implication of $E_L$ and $E_G$ on the scale-up of the bubble column is that, by keeping the gas superficial velocity constant (which is the most critical criterion), a bigger column diameter leads to greater backmixing in both the liquid and gas — that is, greater deviation from PFR characteristics. This is a concern only if the small-scale bubble column behaves like a PFR.

**Heat-transfer coefficient, $h$.** In equations contained in this section, $k_{L}$ is the thermal conductivity of the liquid, $k'_{L}$ is the thermal conductivity of the suspending solid particles, and $\mu_{W}$ is the liquid viscosity near the heat-exchanger wall.

The correlations presented below are applicable for both an internal coil/tube, and a wall jacket. Combining the surface renewal theory of mass transfer and Kolmogoroff’s theory of isotropic turbulence, Deckwer (33) developed an equation which was later modified by Verma (34) to the form shown in Eq. 29.

To apply this equation to slurry mixtures, the liquid properties should be interpreted as follows.

$$\bar{\rho}_{L} = \phi_{S} \cdot \rho_{S} + \phi_{L} \cdot \rho_{L} \quad (30)$$

where $\phi$ is volume fraction.

$$\bar{\mu}_{L} = \mu_{L} \left( 1 + k, \phi_{S} \right) \quad (31)$$

where $k_s = 3 - 5$ (35).

$$\bar{C}_{P} = w_s \cdot C_{P,S} + w_L \cdot C_{P,L} \quad (32)$$

where $w$ is weight fraction.

$$\bar{k}_{L} = \frac{2k_{L} + k_{SL} - 2\phi_{s} \left( k_{SL} - k_{LS} \right)}{2k_{L} + k_{LS} + \phi_{S} \left( k_{LS} - k_{SL} \right)} \quad (33)$$

Joshi and coworkers developed Eq. 34 which is based on the recirculation cell model (36), where $u_{w,ms}$ is the single bubble rise velocity, which can be approximated as 0.265 m/s, read from p. 164 of Ref. 37, or calculated using equations given in Ref. 1, and $u_{w,p}$ is the liquid viscosity near the wall. Obviously, Eq. 34 is more difficult to use than Eq. 29.

The two correlations fit the literature data equally well (1). Equation 34 indicates slight dependence upon column diameter, while it has been reported that column diameter has no effect on $h$ if $d_c > 3$ in. So, Eq. 29 probably is more applicable for industrial-scale columns.

**Note:**
1. $h$ is higher in multiphase flows than in the single-phase (liquid) flow.
2. For Newtonian liquids, $h$ is the same for an internal coil/tube and a wall jacket.
3. For non-Newtonian liquids, an internal coil/tube has higher $h$ than a wall jacket if $u_G < 0.04$ m/s. If $u_G > 0.04$ m/s, there is no difference.

**Equation 29.**

$$\frac{h}{\bar{\rho}_{L} \cdot C_{P,L} \cdot u_G} = 0.121 \left( 1 - e_G \right) \left( \frac{u_{L}^2}{\bar{\mu}_{L} \cdot g} \right)^{-0.25} \left( C_{P,L} \cdot \bar{\mu}_{L} \right)^{-0.50} \quad (34)$$

**Equation 34.**

$$\frac{h \cdot d_c}{k_{L}} = 0.48 \left[ \frac{d_c^{0.33} \cdot g^{0.33} \cdot \left( u_G - e_G \cdot u_{w,ms} \right)^{0.33} \cdot \bar{\mu}_{L}}{\mu_L} \right]^{0.67} \left( C_{P,L} \cdot \bar{\mu}_{L} \right)^{0.33} \left( \frac{\mu_L}{k_{L}} \right)^{0.14} \quad (35)$$

4. Solid suspension elevates $h$. Within practical ranges, $h$ rises with increasing solid concentration and particle size.

**Mechanically agitated tanks**

Mass-transfer coefficient, $k_{a}$. For oxygen (air) and water without electrolytes, the following equation (38) has been shown to correlate most literature data within 40% accuracy:

$$k_{a} = 2.6 \times 10^{-2} \cdot e_{v}^{0.64} \cdot u_{G}^{0.2} \quad (35)$$

with $k_{a}$ in $s^{-1}$, $e_{v}$ (the power dissipation per unit liquid volume) in W/m$^3$, and $u_G$ (the gas superficial velocity) in m/s. The presence of electrolytes in water increases the $k_{a}$ value. It also augments the effect of $e_{v}$ and reduces the effect of $u_G$ on $k_{a}$ that is,

$$k_{a} = 2.0 \times 10^{-3} \cdot e_{v}^{0.2} \cdot u_{G}^{0.2} \quad (36)$$

**Note:**
1. Impeller type and number have little influence on $k_{a}$ as long as $e_{v}$ and $u_G$ are kept constant.
2. The gas sparger should be placed directly beneath the impeller. In case of a ring sparger, its diameter should be slightly less than the impeller diameter.
3. To estimate $k_{a}$ for gas/liquid pairs other than oxygen/water, use either the film or penetration (or surface renewal) theory, whichever gives the more conservative estimate.

**Film theory:**

$$\frac{k_{a}}{D_1} = \frac{D_1}{D_2} \quad (37)$$

Penetration theory:

$$\frac{k_{a}}{D_1} = \sqrt{\frac{D_1}{D_2}} \quad (38)$$

4. In general, $k_{a}$ increases with increasing pressure and temperature, and with decreasing G/L interfacial tension and liquid viscosity.

To establish a $k_{a}$ correlation such as Eq. 35 or Eq. 36, $e_{v}$ is measured from a torque gauge attached to the impeller shaft.
On the other hand, to design a new reactor, $\varepsilon_V$ must be determined before $k_{L}A$ can be calculated. This involves five steps.

1. Determine the value of the impeller’s power number, $Po$. It is a function of the Reynolds number:

$$Re = \frac{D_I \cdot N \cdot d_I^2}{\mu_L}$$  \hspace{1cm} (39)

in which $N$ is the impeller rotational speed in rev/s, and $d_I$ the impeller diameter. $Po$ is constant at $Re > 10^4$. $Po$ curves or values can be found in the literature (for instance, Refs. 13, 39, and 40) for common impellers, but must be obtained from vendors for proprietary impellers.

2. Calculate the impeller’s ungassed power draw, $P_U$, for a single impeller:

$$P_U = Po \cdot \rho_L \cdot N^3 \cdot d_I^5$$  \hspace{1cm} (40)

or via Eq. 41 for multiple impellers.

3. Find the ratio of gassed to ungassed power draw, $P_G/P_U$. This ratio depends upon the gassing rate (as illustrated in Figure 6) and can be found in the literature for common impellers (13). For proprietary impellers, consult vendors.

4. Calculate gassed power draw $P_G = P_U \cdot (P_G/P_U)$  \hspace{1cm} (42)

5. Finally, $\varepsilon_V = P_G/V_L$  \hspace{1cm} (43)

where $V_L$ is the total volume of the liquid.

Other correlations are reviewed in Refs. 13 and 29. For G/L systems other than $O_2$/water, the series of studies by Calderbank et al. (summarized in Refs. 24 and 41) can be applied. In this approach, the liquid-side masstransfer coefficient, $k_L$, and G/L interfacial area, $a$, are estimated separately. It also is assumed $k_{L} = k$, which is valid for most gases but not for vapors. For $k_L$, Eq. 44 applies for $d_G \leq 1$ mm, and Eq. 45 for $d_G \geq 2.5$ mm.

For $1 < d_G < 2.5$ mm, interpolate linearly for $d_G$ between the two equations. These equations are valid for mechanically agitated tanks, as well as bubble and plate columns. The correlations of $\varepsilon_G$, $d_G$, and $a$ for agitated tanks are summarized below.

Gas holdup, $\varepsilon_G$. For air/water, the following equation has been established (42):

$$\varepsilon_G = 0.23 \varepsilon_V^{0.31} \cdot u_G^{0.67}$$  \hspace{1cm} (46)

with $\varepsilon_V$ in W/m$^3$, and $u_G$ in m/s.

The following equations developed by Calderbank and coworkers (24) are applicable for general G/L systems.

For liquids that contain no electrolytes,

$$\varepsilon_G = \left( \frac{u_G \cdot \varepsilon_G}{u_{G_{\text{b}}}} \right)^{0.50} + 0.015 \cdot a$$  \hspace{1cm} (47)

in which $u_{G_{\text{b}}}$ can be approximated as 0.87 ft/s (0.265 m/s), $u_G$ must be in the same unit as $u_{G_{\text{b}}}$, and $a$, as given in Eq. 52, is in cm$^4$.

For solutions of electrolytes,

$$\varepsilon_G = 470 \varepsilon_V^{0.5} \cdot u_{G_{\text{b}}}^{0.6} \cdot \eta^{0.4} \cdot \gamma^{0.4}$$  \hspace{1cm} (48)

where $\varepsilon_V$ is in hpf$^3$, $u_G$ is in ft/s, and $\gamma$ is the liquid specific gravity.

In general, $\varepsilon_G$ rises with pressure.

Bubble diameter, $d_b$ (24). For liquids containing no electrolytes,

$$d_b = 0.0279 \left( \frac{\sigma^{0.6} \cdot \varepsilon_V^{0.5}}{\mu_L^{0.2} \cdot \gamma^{0.2}} \right) + 0.09$$  \hspace{1cm} (49)

For solutions of electrolytes,

$$d_b = 0.0153 \left( \frac{\sigma^{0.6} \cdot \varepsilon_V^{0.4}}{\mu_L^{0.2} \cdot \gamma^{0.2}} \right)^{0.25}$$  \hspace{1cm} (50)

For aqueous solution of alcohols,

$$d_b = 0.013 \left( \frac{\sigma^{0.6} \cdot \varepsilon_V^{0.65}}{\mu_L^{0.25}} \right)$$  \hspace{1cm} (51)

In the above equations, $d_b$ is in cm, $\sigma$ (the G/L interfacial tension) in dyne/cm, and $\varepsilon_V$ in hpf$^3$.

G/L interfacial area, $a$ (24). For liquids containing no electrolytes,

$$a = 215 \left( \frac{\varepsilon_V^{0.4}}{\sigma^{0.6}} \right)^{0.5} \left( \frac{u_G}{u_{G_{\text{b}}}} \right)^{0.5}$$  \hspace{1cm} (52)

where $a$ is in cm$^4$, $\varepsilon_V$ in hpf$^3$, $\sigma$ in dyne/cm, $u_G$ in ft/s, and $u_{G_{\text{b}}}$ can be approximated as 0.87 ft/s (0.265 m/s). Equation 52 gives the G/L interfacial area if surface aeration is negligible, generally when

$$\left( \frac{N \cdot d_I^2 \cdot \rho_L}{\mu_L} \right)^{0.7} \left( \frac{N \cdot d_I^2 \cdot \rho_L}{\mu_L} \right)^{0.3} < 25,000$$  \hspace{1cm} (53)

When surface aeration is significant, the G/L interfacial area is higher than that predicted by Eq. 52. Under such a condition, $a$ calculated by Eq. 52 must be augmented by

$$a = 5 \varepsilon_G/d_b$$  \hspace{1cm} (54)

For liquids containing electrolytes or alcohol, $a$ can be estimated from $d_b$ and $\varepsilon_G$ via:

$$a = \frac{\varepsilon_G}{d_b}$$  \hspace{1cm} (55)

Heat-transfer coefficient, $h$. In equations contained in this section, $k_{L \cdot L}$ is the thermal conductivity of the liquid, $d_G$ is the outside diameter of

---

**Equation 41.**

$$P_U = \rho_L \cdot N^3 \left( P_{O_1} \cdot d_{I_1}^5 + P_{O_2} \cdot d_{I_2}^5 + \ldots + P_{O_n} \cdot d_{I_n}^5 \right)$$

**Equation 44.**

$$k_{L \cdot G} \cdot d_G = 2 + 0.31 \left[ \frac{d_G^3 \cdot (\rho_L - \rho_G) \cdot g}{\mu_L \cdot D_L} \right]^{0.33}$$

**Equation 45.**

$$k_{L \cdot G} \cdot d_G = 0.42 \left[ \frac{\mu_L}{\rho_L \cdot D_L} \right] \left[ \frac{d_G^3 \cdot (\rho_L - \rho_G) \cdot g}{\mu_L \cdot D_L} \right]^{0.33}$$
### Table 6. Values of constants in Eq. 56.

<table>
<thead>
<tr>
<th>Impeller</th>
<th>(a)</th>
<th>(b)</th>
<th>(m)</th>
<th>Range of Reynolds number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Paddle</td>
<td>0.36</td>
<td>0.67</td>
<td>0.21</td>
<td>300-3 \times 10^6</td>
</tr>
<tr>
<td>Pitched-blade turbine</td>
<td>0.53</td>
<td>0.67</td>
<td>0.24</td>
<td>80-200</td>
</tr>
<tr>
<td>Disk, flat-blade turbine</td>
<td>0.55</td>
<td>0.67</td>
<td>0.14</td>
<td>40-3 \times 10^6</td>
</tr>
<tr>
<td>Propeller</td>
<td>0.54</td>
<td>0.67</td>
<td>0.14</td>
<td>2 \times 10^6</td>
</tr>
<tr>
<td>Anchor*</td>
<td>1.0</td>
<td>0.50</td>
<td>0.18</td>
<td>10-300</td>
</tr>
<tr>
<td>Anchor*</td>
<td>0.36</td>
<td>0.67</td>
<td>0.18</td>
<td>300-4 \times 10^6</td>
</tr>
<tr>
<td>Helical ribbon</td>
<td>0.63</td>
<td>0.50</td>
<td>0.18</td>
<td>8-10^5</td>
</tr>
</tbody>
</table>

* Depending upon Reynolds number.

---

For Rushton turbines, Eq. 59 applies for \(10^3 \leq Re \leq 2 \times 10^6\), where \(n_g\) is the number of tubes in one “baffle.”

For the tube side of straight tubes (24) use Eq. 60 where \(d_i\) is the tube inside diameter, and the physical and transport properties are those of the heat-exchange medium. This equation is valid for \(Re \geq 10^4, 0.7 \leq Pr \leq 700\), and the ratio of tube length to \(d_i > 60\).

For the tube side of coils (24):

\[
h_{coil} = h_{straight} \left[ 1 + 3.5 \frac{d_i}{d_h} \right]
\]

where \(d_h\) is the diameter of the coil loop.

### Packed columns

Mass-transfer coefficient — countercurrent. For conventional dumped packings such as Raschig rings, Pall rings, Berl saddles, spheres, and rods, Eq. 62 is recommended (24).

It is a dimensional equation, with \(k_1\) in ft/h (assuming \(k_L = k_1\)), \(\rho_L\) in lb/ft\(^3\), \(\mu_L\) in lb-ft/ft\(^2\)-s, \(g = 4.17 \times 10^6\) ft/ft\(^3\), \(m_L\) (the liquid flux) in lb/ft\(^2\)-h, \(a_w\) (wetted surface area of the packings) in ft\(^2\)/ft\(^3\) (assuming \(a = a_w\) as given below), \(D_i\) in ft/h, \(a_p\) (the external surface of the packing per unit volume of the column; well documented for conventional dumped packings, for instance, in Ref. 24 and 24a) in ft\(^2\)/ft\(^3\), and \(d_s\) (diameter of a sphere having the same external surface as the packing) in ft.

Dimensionless Eq. 63 is used to evaluate \(a_w\). Values of \(\sigma_C\), the critical surface tension of packing material, are given in Table 7.

It is assumed that \(k_1 \cdot a_w\) equals \(k_{eff}\). For air/water, a simpler equation for \(k_1\) is given in Ref. 24.

For special packings, dumped or stacked, the mass-transfer coefficient must be obtained from vendors.

Mass-transfer coefficient — countercurrent, downflow, trickle beds (25). \(k_{eff}\) is correlated with \(\epsilon_v\):

\[
\epsilon_v = \frac{\Delta P_{col}}{H} \cdot u_L
\]
Table 7. Critical surface tension for various packing materials.

<table>
<thead>
<tr>
<th>Packing Material</th>
<th>( \sigma_p ) dyn/cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>56</td>
</tr>
<tr>
<td>Ceramic</td>
<td>61</td>
</tr>
<tr>
<td>Glass</td>
<td>73</td>
</tr>
<tr>
<td>Paraffin</td>
<td>20</td>
</tr>
<tr>
<td>Polyethylene</td>
<td>33</td>
</tr>
<tr>
<td>Polyvinyl chloride</td>
<td>40</td>
</tr>
<tr>
<td>Steel</td>
<td>75</td>
</tr>
</tbody>
</table>

\( \Delta p_{GL} \) is the pressure drop of the two-phase flow over the \( H \) column height, and \( u_L \) is the liquid superficial velocity.

For \( 5 \leq \varepsilon_v < 100 \) W/m\(^3\) (trickle-flow regime),

\[
k_{i,a} = 0.0011 \varepsilon_v \cdot \frac{D_L}{2.4 \times 10^{-9}} \tag{65}
\]

with \( k_{i,a} \) in s\(^{-1}\), and \( D_L \) in m\(^2\)/s. The liquid viscosity effect is included in \( D_L \). For very small gas and liquid velocities, where \( \varepsilon_v < 5 \) W/m\(^3\), use \( k_{i,a} = 0.008 \) s\(^{-1}\).

For \( \varepsilon_v > 100 \) W/m\(^3\) (pulsing and spray flow regimes),

\[
k_{i,a} = 0.0173 \varepsilon_v^{0.5} \cdot \left( \frac{D_L}{2.4 \times 10^{-9}} \right)^{0.5} \tag{66}
\]

Mass-transfer coefficient — countercurrent, upflow, flooded beds (25). If no reliable data are available, use the following rules.

In the bubble flow regime, \( k_{i,a} = 0.15 \) s\(^{-1}\). In the pulse and spray flow regimes, \( k_{i,a} \) could be 20–100% higher than the value for countercurrent downflow at the gas and liquid flow rates. For design purposes, use the

value calculated from Eq. 66.

Gas and liquid holdups. All holdups are expressed as fractions of the volume of the empty column. Total liquid holdup consists of two components — static and dynamic (or operating) holdups:

\[
\varepsilon_{L,T} = \varepsilon_{L,S} + \varepsilon_{L,D} \tag{67}
\]

The static holdup is the liquid fraction that can’t be drained. When the reaction occurs only in the liquid phase, the dynamic holdup is the liquid fraction to accommodate the reaction. The total liquid holdup and the gas holdup should equal the column voidage:

\[
\varepsilon_{L,T} + \varepsilon_G = \varepsilon_C \tag{68}
\]

In countercurrent flow, for the liquid static holdup (24a),

\[
\varepsilon_{L,S} = C_1 \cdot \frac{\mu_L^2 \cdot \sigma_{L,3}^2}{\rho_L^{0.37}} \tag{69}
\]

where \( \mu_L \) is in cP, \( \sigma_L \) in dyne/cm, and \( \rho_L \) in lb/ft\(^3\). Table 8 provides values of \( C_1 \), \( C_2 \), and \( C_3 \) for several packings. For other packings, consult the


For the liquid dynamic holdup (24a), Eq. 70 applies, where \( u_L \) is the liquid superficial velocity, and \( d_p \) is the nominal packing size (or diameter).

For countercurrent, downflow in trickle beds, see the recommendations on pp. 199 of Ref. 25.

For countercurrent, upflow in a flooded bed, see the recommendations on pp. 247 of Ref. 25.

Gas and liquid dispersion coefficients, \( E_L \) and \( E_G \).

For countercurrent flow, considerable disagreement exists in the literature (25). Thus, no recommendations can be given on correlations. Because most studies indicate no column diameter effect, a small column \((d_L/d_p > 8)\) can be used to investigate effects of relevant design and operational variables such as packing size and type, gas and liquid flow rates, and the like. The results can be used to assess the degree of backmixing in the larger column.

For countercurrent, downflow in trickle beds, in the trickle-flow regime (25),

\[
P_{E_L} = 0.042 \cdot R_e_L^{0.5} \tag{71}
\]

and

\[
P_{E_G} = 1.8 \cdot R_e_G^{0.7} \cdot 10^{-0.005 R_{el}} \tag{72}
\]

where

\[
P_{E_L} = \frac{u_L \cdot d_p}{E_L \cdot \varepsilon_L} \tag{73}
\]

\[
P_{E_G} = \frac{u_G \cdot d_p}{E_G \cdot \varepsilon_G} \tag{74}
\]

\[
R_{el} = \frac{\rho_L \cdot u_L \cdot \varepsilon_L}{\mu_L \cdot (1 - \varepsilon_G)} \tag{75}
\]

\[
R_{ef} = \frac{\rho_G \cdot u_G \cdot \varepsilon_G}{\mu_G \cdot (1 - \varepsilon_L)} \tag{76}
\]

Similar information for the pulse and spray flow regimes is not available.

For countercurrent, upflow in flooded beds, the liquid-phase dispersion coefficient (25) is given by Eq. 77.

The value of \( E_L \) in the flooded bed is smaller (that is, there is less backmixing) than that in the unpacked

Equation 63.

\[
\frac{a_w}{a_p} = 1 - \exp \left[ -1.45 \left( \frac{\sigma_c}{\sigma_L} \right)^{0.75} \left( \frac{m_t}{m_p \cdot \mu_L} \right)^{0.1} \left( \frac{m_t^2 \cdot a_p}{\rho_L \cdot g} \right)^{-0.05} \left( \frac{m_t^2}{\rho_L \cdot \sigma_L \cdot a_p} \right)^{0.2} \right]
\]

Equation 70.

\[
\varepsilon_{L,D} = 2.2 \left( \frac{u_L \cdot \mu_L}{d_p \cdot \rho_L \cdot g} \right)^{0.33} + 1.8 \left( \frac{u_L^2}{g \cdot d_p} \right)^{0.50}
\]
### Table 8. Values of constants in Eq. 69.

<table>
<thead>
<tr>
<th>Packing</th>
<th>(C_1)</th>
<th>(C_2)</th>
<th>(C_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-in. carbon Raschig ring</td>
<td>0.086</td>
<td>0.02</td>
<td>0.23</td>
</tr>
<tr>
<td>1-in. ceramic Raschig ring</td>
<td>0.0092</td>
<td>0.02</td>
<td>0.99</td>
</tr>
<tr>
<td>1-in. ceramic Berl saddle</td>
<td>0.0055</td>
<td>0.04</td>
<td>0.55</td>
</tr>
</tbody>
</table>

For other packings and for liquid dynamic holdup, consult Ref. 24a, pp. 14-47.

bubble column under equivalent flow conditions. No correlation is available for \(G\).

**Heat-transfer coefficient.** Packed columns mostly are operated in isothermal or adiabatic mode. Temperature control in the column usually is accomplished by vaporization of the liquid feed stream or additional liquid injected along the length of the column. Heat exchange also can take place outside the column, when the liquid is pumped around the column or pumped through a redistribution depot.

Little information exists on the heat-transfer coefficient in a countercurrent packed column. For trickle beds, information can be found in p. 220 of Ref. 25. A general discussion on heat transfer in gas/liquid/solid reactors appears in Chap. 11 of Ref. 43, and p. 307 of Ref. 44. A good introduction to heat-transfer coefficients in a packed column with single-phase flow is provided on p. 11-28 of Ref. 24a.

**Pipe/tube contactors**

**Mass-transfer coefficient, \(k_{t,a}\).** For horizontal pipes in the bubble or plug flow regimes (15), use Eq. 78, where \(k_{t,a}\) is in \(s^{-1}\), \(u_l\) and \(u_G\) in \(cm/s\), \(\sigma_l\) in \(dyne/cm\), \(\mu_l\) in \(cP\), \(D_l\) in \(cm^2/s\), and \(d_i\) in \(cm\). Note that as the pipe diameter decreases, \(k_{t,a}\) increases significantly. This suggests high \(k_{t,a}\) values in monoliths and membrane hollow fibers. For horizontal pipes in the other flow regimes (15)

for \(\varepsilon_v < 0.05\) atm/s:

\[
k_{t,a} = 3.5D_l^{0.5} \cdot \sigma_l^{0.5} \cdot \mu_l^{0.05} \cdot d_i^{0.68} \cdot \varepsilon_v^{0.4}
\]  

(79)

for \(\varepsilon_v \geq 0.05\) atm/s:

\[
k_{t,a} = 18.7D_l^{0.5} \cdot \sigma_l^{0.5} \cdot \mu_l^{0.05} \cdot \varepsilon_v^{0.8}
\]  

(80)

with the same units as in Eq. 78, except that \(d_i\) is in \(in.\), and \(\varepsilon_v\) in atm/s. The volume-specific power dissipation, \(e_v\), is defined as

\[
e_v = \frac{\Delta P_{GL}}{H} \cdot \left(\frac{u_l + u_G}{u_l + u_G}\right)
\]  

(81)

in which \(\Delta P_{GL}\) is the pressure drop of the two-phase flow over the height or length of the pipe, \(H\).

No correlation is available for \(k_{t,a}\) for vertical pipes.

**Dispersion coefficient.** Liquid dispersion coefficients have been reported for vertical upflow systems (23), but no general correlation is available.

**Heat-transfer coefficient (23).**

For horizontal and vertical pipes in the annular and spray (or mist) flow regimes, Eq. 82 applies.

For horizontal and vertical pipes in the bubble and slug flow regimes:

\[
\frac{h}{H} = 3.4 \left(\frac{X_G}{X_l}\right)^{0.45}
\]  

(83)

where \(h\) is the heat-transfer coefficient based on all liquid flow, that is, from Eq. 60, and \(X_G\) is

\[
X_G = \frac{e_G}{1 - e_G} \left(\frac{\mu_G}{\mu_l}\right)^{0.9} \left(\frac{P_G}{P_l}\right)^{0.5} \left(\frac{\sigma_G}{\sigma_l}\right)^{0.1}
\]  

(84)

**Other types of contactors**

Additional data and correlations are reviewed in Refs. 16 and 23. More details about the venturi/tubular ejector, which is a critical component of the commercial Buss loop reactor, have been published in Refs. 5, 6, and 27. Technical information about the Burdosa jet loop reactor can be found in Refs. 7 and 8, and the impinging zone reactor in Refs. 9 and 45.

**Scale-up design**

Economic viability is the ultimate objective for a commercial reactor. The technical goals in scaling up are to attain desired process results such as blending homogeneity, high product yield, and a short cycle or space time of a batch or continuous process.

Scale-up generally involves one of two approaches:

1. principles of similarity; or
2. mathematical modeling.

The principles of similarity are
### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>G/L interfacial area per unit volume of mixture, m²/m³</td>
</tr>
<tr>
<td>(a')</td>
<td>G/L interfacial area per unit volume of liquid, m²/m³</td>
</tr>
<tr>
<td>(a_p)</td>
<td>External surface area of packings per unit volume of packed column, m²/m³</td>
</tr>
<tr>
<td>(a_w)</td>
<td>Wetted surface area of packings per unit volume of packed column, m²/m³</td>
</tr>
<tr>
<td>(A)</td>
<td>Total surface area for heat exchange, m²</td>
</tr>
<tr>
<td>(Bd)</td>
<td>Bodenstein number of gas flow, defined in Eq. 28</td>
</tr>
<tr>
<td>(Bo)</td>
<td>Bond number, defined in Eq. 14</td>
</tr>
<tr>
<td>(c)</td>
<td>Molar concentration in liquid phase, kg/m³</td>
</tr>
<tr>
<td>(C_p)</td>
<td>Specific heat capacity, J/kg°C</td>
</tr>
<tr>
<td>(d_b)</td>
<td>Bubble diameter, m</td>
</tr>
<tr>
<td>(d_c)</td>
<td>Column diameter, m</td>
</tr>
<tr>
<td>(d_h)</td>
<td>Diameter of helical coil loop, m</td>
</tr>
<tr>
<td>(d_i)</td>
<td>Inside diameter of pipe or tube, m</td>
</tr>
<tr>
<td>(d_I)</td>
<td>Impeller diameter, m</td>
</tr>
<tr>
<td>(d_o)</td>
<td>Outside diameter of pipe or tube, m</td>
</tr>
<tr>
<td>(d_p)</td>
<td>Nominal packing diameter, m</td>
</tr>
<tr>
<td>(d_s)</td>
<td>Diameter of sphere having same external surface area as packing, m</td>
</tr>
<tr>
<td>(d_T)</td>
<td>Tank diameter, m</td>
</tr>
<tr>
<td>(D)</td>
<td>Diffusivity, m²/s</td>
</tr>
<tr>
<td>(E)</td>
<td>Dispersion coefficient, m²/s</td>
</tr>
<tr>
<td>(f)</td>
<td>Fanning friction factor</td>
</tr>
<tr>
<td>(F_p)</td>
<td>Packing factor (see Figure 9), 1/m</td>
</tr>
<tr>
<td>(Ft_o)</td>
<td>Flow number based on (Q_o) in stirred tank = (Q_o/\pi d^2)</td>
</tr>
<tr>
<td>(Fr)</td>
<td>Froude number, defined in Eq. 16</td>
</tr>
<tr>
<td>(g)</td>
<td>Gravitational constant, m/s²</td>
</tr>
<tr>
<td>(g_c)</td>
<td>Unit conversion constant, 9.8 kg/m/s²/10 = 32.2 lb/ft/s²/10</td>
</tr>
<tr>
<td>(G)</td>
<td>Mass of gas flow per unit cross-sectional area of G/L contactor, kg/m³</td>
</tr>
<tr>
<td>(Ga)</td>
<td>Galilei number, defined in Eq. 15</td>
</tr>
<tr>
<td>(h)</td>
<td>Heat-transfer coefficient, W/m²°C</td>
</tr>
<tr>
<td>(H)</td>
<td>Height of vessel, m</td>
</tr>
<tr>
<td>(H_s)</td>
<td>Height of liquid, m</td>
</tr>
<tr>
<td>(Ha)</td>
<td>Ha muster number, per Eq. 3</td>
</tr>
<tr>
<td>(i)</td>
<td>Ionic strength, kg ion/m³</td>
</tr>
<tr>
<td>(k)</td>
<td>Reaction rate constant (see Eq. 2), kg/m³/kg-mole/s</td>
</tr>
<tr>
<td>(k_w)</td>
<td>Constant used in Eqs. 9 and 21</td>
</tr>
<tr>
<td>(k_l)</td>
<td>Liquid-side mass-transfer coefficient, m/s</td>
</tr>
<tr>
<td>(k_{L})</td>
<td>Overall mass-transfer coefficient based on liquid-side concentration differential, m/s</td>
</tr>
<tr>
<td>(k_{La})</td>
<td>Overall mass-transfer coefficient per unit volume of the G/L mixture, 1/s</td>
</tr>
<tr>
<td>(k_i)</td>
<td>Constant in Eq. 31</td>
</tr>
<tr>
<td>(k_i)</td>
<td>Thermal conductivity, W/m°C</td>
</tr>
<tr>
<td>(KE_m)</td>
<td>Head of kinetic energy of gas at inlet to pipe/ring sparger, defined in Eq. 115, m</td>
</tr>
<tr>
<td>(L)</td>
<td>Length of pipe or tube, m</td>
</tr>
<tr>
<td>(m_L)</td>
<td>Liquid flux, lb/h ft²</td>
</tr>
<tr>
<td>(n_p)</td>
<td>Number of tubes in hale</td>
</tr>
<tr>
<td>(N)</td>
<td>Impeller speed, rev/s</td>
</tr>
<tr>
<td>(N_{CD})</td>
<td>Impeller speed at which complete dispersion of gas begins (see Figure 6 and Eq. 7), rev/s</td>
</tr>
<tr>
<td>(N_F)</td>
<td>Impeller speed below which impeller is flooded by gas (see Figure 6 and Eq. 6), rev/s</td>
</tr>
<tr>
<td>(N_p)</td>
<td>Impeller speed at which gross recirculation of gas back into impeller begins (see Figure 6 and Eq. 8), rev/s</td>
</tr>
<tr>
<td>(N_{11})</td>
<td>First normal stress difference, Pa</td>
</tr>
<tr>
<td>(p)</td>
<td>Pressure, Pa</td>
</tr>
<tr>
<td>(p_f)</td>
<td>Pressure drop, Pa</td>
</tr>
<tr>
<td>(p_{G2})</td>
<td>Pressure drop of two-phase flow, m</td>
</tr>
<tr>
<td>(p_{G0})</td>
<td>Head of pressure drop of gas at orifice of sparger, defined in Eq. 117, m</td>
</tr>
<tr>
<td>(p_{Gp})</td>
<td>Head of total pressure drop of gas over length of a sparger, defined in Eq. 116, m</td>
</tr>
<tr>
<td>(P)</td>
<td>Power, W or kW</td>
</tr>
<tr>
<td>(P_e)</td>
<td>Pelet number, defined in Eqs. 73 and 74</td>
</tr>
<tr>
<td>(P_{G})</td>
<td>Power number of impeller = (P/(\rho_{G}N_{11}d^{3}))</td>
</tr>
<tr>
<td>(P_{G0})</td>
<td>Gassed power drop in stirred tank, W</td>
</tr>
<tr>
<td>(P_{G1})</td>
<td>Ungassed power drop in stirred tank, W</td>
</tr>
<tr>
<td>(Q)</td>
<td>Volumetric flow rate, m³/s</td>
</tr>
<tr>
<td>(Q_{G})</td>
<td>Heat-exchanger duty or total reaction heat, J/s</td>
</tr>
<tr>
<td>(r)</td>
<td>Reaction rate per unit volume of G/L mixture, kg-mole/m³</td>
</tr>
<tr>
<td>(Re)</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>(Sc)</td>
<td>Schmidt number, defined in Eq. 13</td>
</tr>
<tr>
<td>(SF)</td>
<td>Scale-up factor</td>
</tr>
<tr>
<td>(Sh)</td>
<td>Sherwood number, defined in Eq. 12</td>
</tr>
<tr>
<td>(t)</td>
<td>Gas average residence time = (V_o/n_p), s</td>
</tr>
<tr>
<td>(t_{mix})</td>
<td>Mixing time in stirred tank, s</td>
</tr>
<tr>
<td>(T)</td>
<td>Temperature, °C</td>
</tr>
<tr>
<td>(u)</td>
<td>Superficial velocity of gas or liquid in G/L contactor, m/s</td>
</tr>
<tr>
<td>(u_{wp})</td>
<td>Rise velocity of single bubble = 0.265 m/s = 0.87 ft/s</td>
</tr>
<tr>
<td>(u_{G})</td>
<td>Rise velocity of bubble swarm, m/s</td>
</tr>
<tr>
<td>(U)</td>
<td>Overall heat-transfer coefficient, W/m²°C</td>
</tr>
<tr>
<td>(V_{G})</td>
<td>Volume of G/L mixture in contactor, m³</td>
</tr>
</tbody>
</table>

### Greek Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\alpha)</td>
<td>Constant used in Eq. 115</td>
</tr>
<tr>
<td>(\beta)</td>
<td>Volume ratio of liquid to liquid-side diffusion films, defined in Eq. 4</td>
</tr>
<tr>
<td>(\gamma)</td>
<td>Specific gravity</td>
</tr>
<tr>
<td>(\gamma_{eq})</td>
<td>Effective shear rate of non-Newtonian liquid, defined in Eq. 20/13</td>
</tr>
<tr>
<td>(\delta)</td>
<td>Thickness of liquid-side diffusion films, m</td>
</tr>
<tr>
<td>(\varepsilon_c)</td>
<td>Voidage of packed column</td>
</tr>
<tr>
<td>(\varepsilon_{G})</td>
<td>Gas holdup</td>
</tr>
<tr>
<td>(\varepsilon_L)</td>
<td>Liquid holdup</td>
</tr>
<tr>
<td>(\varepsilon_{L,D})</td>
<td>Dynamic liquid holdup in packed column</td>
</tr>
<tr>
<td>(\varepsilon_{L,S})</td>
<td>Static liquid holdup in packed column</td>
</tr>
<tr>
<td>(\varepsilon_{L,T})</td>
<td>Total liquid holdup in packed column</td>
</tr>
<tr>
<td>(\varepsilon_m)</td>
<td>Power dissipation per unit liquid mass, W/kg</td>
</tr>
<tr>
<td>(\varepsilon_{v})</td>
<td>Power dissipation per unit liquid volume, W/m³</td>
</tr>
<tr>
<td>(\theta)</td>
<td>Space time, s</td>
</tr>
<tr>
<td>(\lambda)</td>
<td>Defined in Figure 10</td>
</tr>
<tr>
<td>(\mu)</td>
<td>Viscosity, kg/m·s, or cp</td>
</tr>
<tr>
<td>(\mu_{L,ef})</td>
<td>Effective viscosity of non-Newtonian liquid, defined in Eq. 19, kg/m·s, or cp</td>
</tr>
<tr>
<td>(\mu_w)</td>
<td>Viscosity of fluid near heat-exchanger wall, kg/m·s, or cp</td>
</tr>
<tr>
<td>(\rho)</td>
<td>Density, kg/m³</td>
</tr>
<tr>
<td>(\sigma)</td>
<td>GL interface tension, kg/s², or dyn/cm</td>
</tr>
<tr>
<td>(\sigma_c)</td>
<td>Critical surface tension, kg/s², or dyn/cm</td>
</tr>
<tr>
<td>(\tau_{eq})</td>
<td>Effective shear stress of non-Newtonian liquid, defined in Eq. 18, kg/m²</td>
</tr>
<tr>
<td>(\phi)</td>
<td>Volume fraction</td>
</tr>
<tr>
<td>(\Phi)</td>
<td>Defined in Eq. 26</td>
</tr>
<tr>
<td>(\Psi)</td>
<td>Defined in Figures 9 and 10</td>
</tr>
</tbody>
</table>

### Subscripts

<table>
<thead>
<tr>
<th>Subscript</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>air</td>
<td>Air</td>
</tr>
<tr>
<td>dissolved</td>
<td>Dissolved gas</td>
</tr>
<tr>
<td>comp</td>
<td>Component originally in liquid</td>
</tr>
<tr>
<td>gas</td>
<td>Gas</td>
</tr>
<tr>
<td>heat</td>
<td>Heat or heat-exchange medium</td>
</tr>
<tr>
<td>at inlet</td>
<td>At inlet</td>
</tr>
<tr>
<td>liquid</td>
<td>Liquid</td>
</tr>
<tr>
<td>at orifice</td>
<td>At orifice</td>
</tr>
<tr>
<td>solid</td>
<td>Solid</td>
</tr>
<tr>
<td>tank</td>
<td>Tank</td>
</tr>
<tr>
<td>water</td>
<td>Water</td>
</tr>
</tbody>
</table>
based on the premise that, if the rules of similarity are met, a large-scale reactor will perform the same, in terms of the technical goals, as a small-scale one. This approach does not involve complicated calculation, nor does it predict the reactor performance. Mathematical modeling, on the other hand, is capable of predicting the reactor performance, but requires more fundamental knowledge about the reaction system. Whole or parts of the similarity method are widely used, but mathematical modeling is less common because it is more demanding.

**Principles of geometric, kinematic, and dynamic similarity**

Geometric similarity requires that all independent ratios of key linear dimensions are identical between the large-scale and small-scale reactors. If the number of key linear dimensions for each reactor is \( n \), then there are \( n - 1 \) independent ratios. For a batch process, the volume of the large-scale reactor poses an additional constraint for the selection of the linear dimensions. For a continuous process, an additional constraint comes from the space time requirement, which is a component of dynamic similarity.

Kinematic similarity demands that the two reactors operate in the same flow regime. This requirement imposes one constraint on all the design variables that influence the flow regime.

Dynamic similarity refers to causes and their effects. The causes involve design variables and mechanisms through which they influence the effects. The effects require that, in different scales, the same cycle or space time produces identical process results. There has been ongoing debate about what criteria should be included to account for dynamic similarity (40, 46). In reactor scale-up, similarity in the following parameters must be maintained.

- **Space time.** This represents the reaction kinetics or the consequence of the interaction between the reaction kinetics and the G/L mass transfer. It imposes a constraint on design variables for a continuous process. For a semi-batch process, the equivalent factor is the batch cycle time; fixing the cycle time removes it as a design variable.

- **Stoichiometric ratio of the liquid-phase reactant to the gas-phase reactant.** The reactant concentrations to be used in scale-up should be maintained. In this case, the stoichiometric ratio is reduced to the ratio of the liquid stock or feed rate to the gas feed rate.

  - **Driving force for the mass transfer, \( \Delta C \).** This is the concentration differential of the dissolved gas between the G/L interface and the liquid bulk. This requirement is satisfied if \( p, T \), and the gas feed concentration are fixed when the reactor scale changes. If these conditions cannot be fixed, mass-balance calculation and Henry’s law must be applied to select \( p, T \), and the gas feed concentration.

  - **\( k_{L}a \).** This is the “conductivity” (that is, the reciprocal of the “resistance”) for the mass transfer. The mass transfer is determined by \( k_{L}a \) and \( \Delta C \). If both \( k_{L}a \) and \( \Delta C \) are identical between the two reactors, the mass-transfer rate per unit volume will be the same.

  - **\( \varepsilon_{G} \).** The gas holdup influences the gas space time. For a continuous process, it also affects the liquid volume where the reaction take place. This requirement usually does not introduce an additional constraint, as \( \varepsilon_{G} \) and \( k_{L}a \) both depend upon the same group of design variables.

- **Heat exchange.** As will be shown later, the heat-exchanger area cannot be scaled up to the same proportionality as the reactor capacity. Therefore, in the large-scale reactor, more demands are placed on the heat-exchange medium.

In spite of the sound rationale behind similarity principles, uncertainty still arises for two reasons:

1. Different opinions exist about what constitutes dynamic similarity, which is the heart of the similarity principles; and

2. Often, there are more constraints than design variables (as will be demonstrated by two examples in the following sections). To come up with a design, some constraints, usually those of the geometric similarity, must be relaxed. It takes experience and judgment to relax constraints without materially affecting the scale-up. It is helpful to supplement the similarity principles by mathematical modeling whenever possible.

**A bubble column**

A small bubble column has been tested to meet conversion and yield targets. The following data on that column are available:

- \( d_{C,small} \), column diameter;
- \( H_{small} \), column height;
- \( Q_{G,small} \), heat-exchange duty;
- \( u_{G,small} \), gas superficial velocity;
- \( Q_{G,small} \), volumetric flow rate of gas; — this is not an independent factor, because

\[
Q_{G,small} = \frac{(\pi/4)}{d_{C,small}^2} u_{G,small} \tag{85}
\]

- \( V_{R,small} \), reactor volume — this is not an independent factor, because

\[
V_{R,small} = \frac{(\pi/4)}{d_{C,small}^2} H_{small} \tag{86}
\]

and \( \theta_{L} \), liquid space time,

\[
\theta_{L} = \frac{V_{R,small}}{Q_{L,small}} \tag{87}
\]

(86) For a continuous process

Based on these data, the reactor is to be scaled up by a factor \( SF \).

For a batch process,

\[
SF = \frac{V_{R,large}}{V_{R,small}} \tag{88}
\]

For a continuous process,

\[
SF = \frac{Q_{L,large}}{Q_{L,small}} \tag{89}
\]

Variables to be specified for the scale-up design are \( d_{C,large}, H_{large}, \) and \( Q_{G,large} \). The large-scale operation will process the same gas and liquid; thus, all the fluid physical and transport property constants remain unchanged. According to dynamic simi-
larity, pressure, temperature, gas feed concentration, and the concentration of the liquid-phase reactant will be the same as those of the small-scale test. Hence, there are only three design variables.

**Geometric similarity constraints.**

\[ H_{\text{large}}/d_C,\text{large} = H_{\text{small}}/d_C,\text{small} \]  
\[ \pi \frac{d_C^2}{4} \cdot H_{\text{large}} = SF \cdot V_{R,\text{small}} \]  

**Kinematic similarity constraints.** Flow regime in the bubble column depends upon the column diameter and the gas superficial velocity, as illustrated in Figure 5. This requirement can be represented by one equation containing all three design variables. Further examination of the flow map reveals that if the gas superficial velocity is maintained constant, the same flow regime will be obtained. Because the constancy of \( u_G \) also is required for dynamic similarity, the constraint equation is not introduced here. However, to avoid slug flow,

\[ d_C,\text{large} > 0.15 \text{ m} \]  

**Dynamic similarity constraints.**

\[ \frac{\pi}{4} \frac{d_C^2,\text{large} \cdot H_{\text{large}}}{Q_{L,\text{large}}} \]  

Depending on whether the process is semi-batch or continuous, either Eq. 91 or Eq. 93 is used.

**Stoichiometry.**

\[ Q_{G,\text{large}} = SF \cdot Q_{G,\text{small}} \]  

**Mass transfer and gas holdup.** Examination of Eqs. 9 and 21 reveals that \( k_f a \) and \( e_G \) will be the same as in the small-scale reactor if \( u_G \) is kept the same, because all the fluid properties are constant. This requirement is met if

\[ u_{G,\text{small}} = \frac{4}{\pi} \frac{Q_{G,\text{large}}}{d_C^2,\text{large}} \]  

In summary, four equality constraints and one inequality constraint are imposed on three design variables. Obviously, it may not be possible to have one design that satisfies all the constraints.

To solve the problem, some equality constraints can be changed to inequality ones, but the changes should be conservative. For example, Eq. 94 can be changed to

\[ Q_{G,\text{large}} \geq SF \cdot Q_{G,\text{small}} \]  

Then, the remaining three inequality constraints are used to solve for \( d_C,\text{large}, H_{\text{large}}, \) and \( Q_{G,\text{large}}; \) the solutions are checked against Eqs. 92 and 96. If the inequality constraints also are satisfied, a reliable scale-up design results. If not, more constraints must be relaxed, but always in the conservative direction, until an acceptable design is achieved.

**Points to consider:**

1. The effect of backmixing (that is, axial dispersion) is not considered in dynamic similarity. Equations 25 and 27 show that both the liquid- and gas-flow dispersion coefficients increase with increasing column diameter and gas superficial velocity. Therefore, if the small reactor has significant PFR characteristics, the large reactor will lose a certain degree of PFR performance. This implies that, if the reaction is of positive order, reactant conversion and product yield will be compromised. One remedy is to extend the batch cycle time or the liquid space time.

2. Gas space time and residence time are not considered in dynamic similarity. The gas space time

\[ t_G = H_{\text{large}}/\dot{u}_G \]  

is longer in the large reactor, as \( H \) is higher but the gas bubble rise velocity, \( \dot{u}_G \), is independent of the reactor size. If the gas absorption is near complete in the small reactor, there is a higher probability that the gas component could be depleted before the bubbles rise to the top of the large reactor. Therefore, it has been suggested that, in scaling up the reactor, \( H/d_C \) be progressively reduced (41). This argument also applies to the mechanically agitated tanks.

**A mechanically agitated tank**

To scale up a small-scale reactor with impeller, the following data are available:

\[ d_{I,\text{small}}, \text{ impeller diameter; } \]
\[ d_{I,\text{large}}, \text{ tank diameter; } \]
\[ H_{\text{small}}, \text{ tank height; } \]
\[ u_{G,\text{small}}, \text{ gas superficial velocity; } \]
\[ Q_{H,\text{small}}, \text{ heat-exchange duty; and } \]
\[ e_{m}, \text{ or } e_{v}, \text{ mass- (liquid) or volume- specific power consumption. } \]

From these, one can find \( V_{R,\text{small}} \) using Eq. 86 for a flat-bottom tank, replacing \( d_C \) with \( d_I \), or

\[ V_{R,\text{small}} = \frac{\pi}{4} d_I^2 \cdot H_{\text{small}} - 0.051 d_I^3 \]  

for a round-bottom tank. Similarly, one obtains \( Q_{G,\text{small}} \) from Eq. 85, and \( \theta_t \) from Eq. 87.

Note that both \( e_m \) and \( e_v \) are functions of \( d_I, d_C, H, \) and \( N \). Either one, or \( N \) can be used as an independent variable, along with \( d_I, \) \( d_C, \) and \( H. \)

For scale-up, Eq. 88 is used for a batch process, and Eq. 89 for a continuous one. Scale-up design variables are \( d_C, \) \( d_I, \) \( H_{\text{large}}, \) \( N_{\text{large}}, \) \( Q_{H,\text{large}}, \) \( \dot{u}_G, \) \( \dot{u}_L, \) and \( Q_{G,\text{large}}. \) For the stirred tank, besides the three geometric dimensions listed above, there are others, such as impeller clearance and baffle width. For each additional dimension, however, there is exactly one additional constraint due to the geometric similarity. Hence, it suffices to include the three dimensions that also are pertinent to flow pattern and transport coefficients. As in the previous example, \( p, T, \) gas feed concentration, liquid-phase reactant feed concentration, and all fluid properties remain unchanged.

**Geometric similarity constraints.**

\[ d_{I,\text{large}}/d_{I,\text{large}} = d_{I,\text{small}}/d_{I,\text{small}} \]  

\[ H_{\text{large}}/d_{I,\text{large}} = H_{\text{small}}/d_{I,\text{small}} \]  

\[ \frac{\pi}{4} d_I^2 \cdot H_{\text{large}} = SF \cdot V_{R,\text{large}} \]  

assuming a flat-bottom tank

**Kinematic similarity constraints.** Equations 6–8 illustrate that flow pattern depends upon \( d_I, d_C, N, \) and \( Q_G; \)

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Although multiple equations need to be evaluated to determine the flow pattern, the same flow pattern requirement can be represented by one equation, namely

$$f_F (d_{L, large}, d_{F, large}, N_{large}, Q_{G, large}) \geq 0$$  \hspace{1cm} (103)

This is an inequality constraint, because a flow pattern corresponds to a range of values of the design variables, not a single set of the values.

**Dynamic similarity constraints.**

$$\theta_L = \frac{\pi d_{F, large}^2 \cdot H_{large}}{Q_{L, large}}$$  \hspace{1cm} (104)

Depending upon whether the process is semi-batch or continuous, either Eq. 102 or Eq. 104 is used.

**Stoichiometry.** Use Eq. 94.

**Mass transfer and gas holdup.** Examination of Eqs. 35 and 46 reveals that $k_F a$ and $\varepsilon_G$ in the small-scale and large-scale reactors will be the same if $e_V$ and $u_c$ are kept the same. As discussed above, evaluation of the power dissipation takes many steps and requires information about the power number and power curve for the particular impeller type. Nonetheless, the criterion of the same $e_V$ can be represented by one equality constraint equation

$$f_F (d_{L, large}, d_{F, large}, N_{large}, Q_{G, large}) = 0$$  \hspace{1cm} (105)

For the requirement of the same gas superficial velocity

$$u_{G, small} = \frac{4 Q_{G, large}}{\pi d_{F, large}^2}$$  \hspace{1cm} (106)

There are six equality and one inequality constraints imposed on five design variables. Again, the number of the constraints is greater than the degrees of design freedom. Conservative adjustment of some constraints is necessary to reach a reliable scale-up design.

**Keep in mind:**

1. To hold the specific power dissipation constant, roughly $N \propto d_{L}^{-0.67}$, in the large reactor, the Reynolds number will be higher, the Froude number lower, the impeller tip speed greater, and the surface aeration more significant (41). This illustrates that, for $k_F a$, keeping the conventional dimensionless groups constant may not be a good scale-up method, and maintaining the impeller tip speed constant is not sufficient.

2. Mixing time, $t_{mix}$, is the time taken to reach homogeneity of the concentration in the stirred tank. It is a measure of mixing effectiveness or quality. To keep $t_{mix}$ constant in geometrically similar tanks, total power required, $P_t \propto d_t^{4.1-3.95}$ (41). Therefore, if the specific power dissipation is maintained at scale-up, that is, $P \propto d_t$, mixing quality will suffer in the large tank. Finally, if $t_{mix}$ is close to $\theta_L$, it is safer to scale up the reactor based on $t_{mix}$ instead of $k_F a$ and $\varepsilon_G$.

### A heat exchanger

Reaction heat is directly proportional to reactor capacity. Thus, the heat balance in the large reactor is

$$U \cdot A \cdot \Delta T = SF \cdot Q_{H, small}$$  \hspace{1cm} (107)

where $U$ is the overall heat-transfer coefficient, $A$ is the total surface area for heat exchange, and $\Delta T$ is the temperature differential between the reactor and the heat-exchange medium. The scale-up factor, $SF$, is based on reactor volume for a batch process, or liquid feed rate for a continuous process. Hence, for geometrically similar reactors,

$$SF \propto d_{c}^3$$  \hspace{1cm} (108)

The heat exchanger can have a wall jacket or immersed coils or tubes. The total surface area is proportional to the product of vessel diameter and height, i.e.,

$$A \propto d_{c}^2$$  \hspace{1cm} (109)

The overall heat-transfer coefficient, $U$, is bound by the vessel-side coefficient, $h$. So, consider the effect of the reactor scaleup on $h$. For the bubble column, Eq. 29 shows that for either type of heat exchanger,

$$h \propto u_{G}^{-0.25}$$  \hspace{1cm} (110)

Because $u_{G}$ is kept constant in the scale-up design, $h$ remains unchanged in the large reactor.

For the stirred tank, recall that by keeping the specific power dissipation constant in the scale-up,

$$N \propto d_{L}^{-0.67} \propto d_{C}^{-0.67}$$ in geometrically similar tanks. According to Eqs. 56–58, the following relationships hold:

For a jacketed heat-exchanger,

$$h \propto d_{C}^{-0.11}$$  \hspace{1cm} (111)

For helical coils,

$$h \propto d_{C}^{-0.39}$$  \hspace{1cm} (112)

For baffle-type tubes,

$$h \propto d_{C}^{-0.67}$$  \hspace{1cm} (113)

This analysis reveals that, as the scale goes up, the heat-transfer efficiency of the wall jacket declines, while that of the helical coils and the baffle-type tubes rises. The baffle-type tube heat exchanger is more favorable than the helical coils because of its greater increase in $h$.

In summary, the product of $A$ and $U$ is proportional to the linear scale of the reactor to a power less than three. To satisfy Eq. 107, $\Delta T$ in the large reactor must be greater than that in the small reactor. This means that the flow rate of the heat-exchange medium must be raised by a factor larger than $SF$, or the temperature of the medium should be decreased for exothermic reactions and increased for endothermic ones. The conditions of the medium can be defined by simultaneously solving Eq. 107 and the following equation.

$$\rho_H \cdot C_{PH} \cdot Q_H \cdot (T_{H, in} - T_{H, out}) = SF \cdot Q_{H, small}$$  \hspace{1cm} (114)

The subscript $H$ represents the heat-exchange medium. $\Delta T$ is the logarithmic mean of the temperature differences at the inlet and outlet between the reactor and the medium.

Note that if the heat exchanger in the small reactor does not make full use of the reactor space, it may be feasible to increase $A$ in the large reactor beyond the level dictated by Eq. 109. In such a case, Eq. 107 could be satisfied without changing the temperature of the heat-exchange medium.
Literature Cited


Mathematical modeling

Mathematical equations, based on mass- and energy-balance principles, can be written to describe chemical and physical processes taking place in a reactor. These equations form a model that enables reactor outputs to be related to geometrical aspects and operating conditions of the reactor. Owing to its quantitative prediction capability, mathematical modeling makes it possible to optimize the scale-up design for a given objective that is a function of inputs to and outputs from the model.

Depending upon how comprehensive and accurate the model needs to be, it invokes various basic laws of thermodynamics, reaction kinetics, and transport phenomena. With a simple reactor model, it may be possible to directly solve for design variables, given reactor performance targets. In contrast, in an advanced, more complex model, a design is specified, and the reactor outputs are found. Thus, iterations are necessary to obtain a final design that meets the performance targets.

A preferred approach to scale up a reactor is to use similarity principles to get a preliminary design, and then apply mathematical modeling to check and refine the design. Simple design equations for various G/L reactors can be found in Ref. 23. Advanced modeling is beyond the scope of this article. Several commercial process-simulation packages contain modules for modeling packed and tray columns via rate- or equilibrium-based approaches.

Other rules of thumb

Gas sparger design

Porous plates and perforated pipes/rings commonly are used as gas spargers. Porous plates can generate fine bubbles at the expense of high pressure drop. Pore sizes usually range from 10 to 100 microns. At high gassing rate, bubble coalescence starts a short distance above the porous plate. Therefore, porous plates are effective only for gassing rates below a certain level expressed as volumetric rate per unit cross-sectional area of the plate.

When selecting a porous plate, it is important to find out from vendors the gassing-rate limit and the pressure-drop characteristics. Porous plates are useful for a bubble column when the gas superficial velocity is lower than 3 cm/s; they offer no advantage in the churn-turbulent flow regime, and are rarely used in the agitated tank.

A critical goal for designing a perforated pipe is to maintain equal flow through each orifice. To check this, three factors must be calculated.

1. Kinetic energy of the gas at the inlet of the pipe,

\[ KE_{in} = \frac{\alpha \cdot u_{in}^2}{2 g_c} \]  \hspace{1cm} (115)

where \( u_{in} \) is the gas inlet velocity, and \( \alpha = 1.05 \) for turbulent flow, or \( \alpha = 2 \) for laminar flow.

2. Total pressure loss along the pipe,

\[ \Delta P_r = \left( \frac{4 f \cdot L}{3 d_i} - 1 \right) \frac{u_{in}^2}{2 g_c} \]  \hspace{1cm} (116)

where \( f \) is the Fanning friction factor, \( L \) the pipe length, and \( d_i \) the pipe inside diameter.

3. Pressure loss across each orifice,

\[ \Delta P_o = \frac{u_o^2}{2 g_c \cdot C_o} \]  \hspace{1cm} (117)

where \( u_o \) is the gas velocity at the orifice assuming equal distribution of the gas feed to each orifice, and \( C_o \) is the orifice coefficient, \( C_o \approx 0.8 \).

To ensure even flow through each orifice, the following criteria must be met (24a):

\[ KE_{in}/\Delta P_o \leq 0.1 \]  \hspace{1cm} (118)

\[ \Delta P_r/\Delta P_o \leq 0.1 \]  \hspace{1cm} (119)

Other rules of thumb (24a,31) include:

\[ u_o \leq 250-300 \text{ ft/s} \]  \hspace{1cm} (120)

\[ Re_o \equiv \text{Reynolds number of gas flow at orifice} \geq 6,000 \]  \hspace{1cm} (121)

More rules of thumb

Bubble columns.

- \( d_c > 0.15 \text{ m} \), to avoid the slug-flow regime for low-viscosity liquids, and to have \( k_{st} \text{ and } k_i \) independent of column diameter;

- \( 3 \leq H_l/d_c \leq 12 \); and

- Height for G/L disengagement = \( 0.75 d_c \), if \( d_c \geq 4 \text{ ft} \), or 3 ft, if \( d_c < 4 \text{ ft} \). **Mechanically agitated tanks.**

- G/L disengagement = \( 0.25 \text{ for Rushton turbines, or } 0.3-0.5 \text{ for other impellers; } \)

- \( H_l/d_r = 1 \); and

- If \( H_l/d_r \geq 2 \), use multiple impellers with the spacing roughly equal to the tank diameter.

Packed columns.

- With dumped packings, the nominal size of the packings should be no less than \( ¼ \text{ in} \). If the packings are catalyst particles, the nominal size should be no less than \( ¼ \text{ in} \); \( d_c/d_p \geq 8 \) at least, with > 30 preferred to prevent liquid channeling;

- Include liquid redistribution device every 10-15 ft packing height; and

- To achieve good wetting of the packings in a trickle bed, \( u_c \geq 1 \text{ cm/s} \). **Jetectors/motionless mixers.**

- \( Q_i/Q_t \equiv 1 \) at the nozzle.

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