

SUPPLEMENTAL MATERIAL

ANNEX I. CORRELATIONS

Minimum fluidization velocity and terminal velocity:

According to Leva [1960]:

$$u_{mf} = 1.118 \cdot 10^{-13} \frac{d_p^{1.82} (\rho_s - \rho_g)^{0.94}}{\rho_g^{0.06} \mu^{0.88}} \quad (83)$$

A more general quadratic expression for u_{mf} follows from equating the pressure drop over the bed at minimum fluidization conditions to the hydrostatic pressure of the bed. Kunii and Levenspiel [1991] show that for small particles and $Re_{p,mf} < 20$ the general expression reduces to:

$$u_{mf} = \frac{d_p^2 (\rho_s - \rho_g) g \varepsilon_{mf}^3 \phi_s^2}{150 \mu (1 - \varepsilon_{mf})} \quad (84)$$

To explicitly account for polydispersity, some empirical correlations can be found in the literature. Kumar and Sen Gupta [1974] carried out pressure drop tests with single, binary, tertiary and quaternary particle mixtures and proposed:

$$u_{mf} = 0.0054 \mu \frac{\overline{Ar}^{0.78}}{\overline{d}_p \rho_f} \quad (85)$$

with the Archimedes number defined by Eq. (58).

In Eq. (85), \overline{Ar} , is to be calculated with the arithmetic mean solids' density and the harmonic mean particle diameter [Yang, 2003]:

$$\overline{\rho}_p = \sum_{i=1}^n \rho_{pi} \quad (86)$$

$$\overline{d}_p = 1 / \sum_{i=1}^n \frac{w_i}{d_{pi}} \quad (87)$$

The terminal velocity of the particles can be obtained by balancing the drag force and the gravity force exerted on a (spherical) particle:

$$u_t = \sqrt{\frac{4g d_p (\rho_s - \rho_g)}{3 \rho_g C_D}} \quad (88)$$

C_D is the drag coefficient and a function of the particle Reynolds number, $Re_p = d_p \rho_g u_t / \mu$.

For a spherical particle and $Re_p < 0.4$ (laminar flow):

$$C_D = 24/Re_p \quad (89)$$

For $1 < Re_p < 10^3$, Trambouze et al. [1984] derived the following expression from experimental data:

$$\ln C_D = -5.150 + \frac{69.43}{\ln Re_p + 7.99} \quad (90)$$

For $Re_p > 10^3$ the flow is fully turbulent and: $C_D = 0.43$.

Haider and Levenspiel [1989] experimentally derived a general expression for the drag coefficient:

$$C_D = \frac{24}{Re_p} \left[1 + (8.1716e^{-4.0655\phi_s}) Re_p^{0.0964+0.5565\phi_s} \right] + \frac{73.69(e^{-5.0748\phi_s}) Re_p}{Re_p + 5.378e^{6.2122\phi_s}} \quad (91)$$

which, for spherical particles, reduces to:

$$C_D = \frac{24}{Re_p} + 3.3643 Re_p^{0.3471} + \frac{0.4607 Re_p}{Re_p + 2682.5} \quad (92)$$

Kunii and Levenspiel [1991] recommend using the average particle diameter for the calculation of u_{mf} . For the calculation of u_t it is recommended to use the smallest diameter for which a substantial fraction is present in the particle size distribution.

Minimum velocity for bubbling:

With Geldart B type particles (e.g. sand particles) [Geldart, 1973], bubbling starts simultaneously with the fluidization of the bed. With smaller Geldart A type particles (e.g. FCC catalyst), uniform fluidization is possible in a small velocity range before bubbling starts. A correlation for the minimum superficial gas velocity required for the formation of bubbles u_{mb} was derived by Geldart and Abrahamsen [1978] from experiments with 23 types of particles ($d_p = 20 - 72 \mu m$, $\rho_s = 1100 - 4600 \text{ kg/m}^3$):

$$\frac{u_{mb}}{u_{mf}} = \frac{4.125 \cdot 10^4 \rho_g^{0.1} \mu^{0.9}}{(\rho_s - \rho_g) g d_p} \quad (93)$$

, where the constant has dimensions $m^{0.2}/s^{1.1}$. Equation (93) was found to correctly predict $u_{mb} < u_{mf}$ for Geldart B and D (e.g. grain) type particles, whereas $u_{mb} \geq u_{mf}$ for fine, Geldart A type particles [Yang, 2003]. It was also observed that the ratio u_{mb}/u_{mf} strongly depends on the weight

fraction of particles with a diameter smaller than 45 μm , $P_{45\mu\text{m}}$, leading to a modified criterion

[Abrahamsen and Geldart, 1980]:

$$\frac{u_{mb}}{u_{mf}} = \frac{2300\rho_g^{0.126}\mu^{0.523}\exp(0.716P_{45\mu\text{m}})}{d_p^{0.8}g^{0.934}(\rho_s-\rho_g)^{0.934}} \quad (94)$$

Bubble volume fraction and bubble rise velocity:

For the calculation of the volume fraction of bubbles in the bed, a good estimate with Geldart A type particles is based on the assumption that any gas fed in excess of the gas that is needed to achieve minimum fluidization enters into the bubble phase, so that the (superficial) emulsion gas velocity is:

$$\varepsilon_e(1 - f_b)u_e = u_{mf} \quad (95)$$

and the volume fraction bubbles in the bed becomes:

$$f_b = \frac{(u_s - u_{mf})}{u_{br}} \quad (96)$$

According to Werther [1978], among a swarm of bubbles, the bubble rise velocity, u_{br} , can be calculated from:

$$u_{br} = \Psi\sqrt{d_b g} \quad (97)$$

where Ψ depends on the tube diameter, d_t :

$$\Psi = 0.64 \quad \text{for } d_t < 0.1\text{m}$$

$$\Psi = 1.6d_t^{0.4} \quad \text{for } 0.1 < d_t < 1.0\text{m} \quad (98)$$

$$\Psi = 1.6 \quad \text{for } d_t > 1.0\text{m}$$

Note that for a single bubble, $\Psi = 0.711$.

The bubble diameter, d_b , evolves with the axial distance from the distributor in the column, z – see Eqs. (4) and (5). It is typically assumed that the void fraction in the emulsion phase equals the void fraction of the bed at minimum fluidization conditions, $\varepsilon_e = \varepsilon_{mf}$. The volume fraction emulsion gas in the bed can then be calculated from:

$$f_e = \varepsilon_{mf}(1 - f_b) \quad (99)$$

Considering the void fraction in the bubble phase is one, the average void fraction or gas hold-up of the bed is then:

$$\varepsilon = f_b + (1 - f_b)\varepsilon_{mf} \quad (100)$$

Some variation of the gas flow rate through the emulsion phase (so different from u_{mf}) and of the emulsion phase void fraction (so different from ε_{mf}) was observed by Abrahamson and Geldart [1980]. No widely applicable relation is available, and variations are only expected to be significant when fluidizing larger particles [Hillgardt and Werther, 1986], typically not of interest for studying intrinsic reaction kinetics. For Geldart A and AB type particles, Abrahamson and Geldart [1980] found the following relations:

$$\left(\frac{\varepsilon_e}{\varepsilon_{mf}}\right)^3 \left(\frac{1-\varepsilon_{mf}}{1-\varepsilon_e}\right) = \left(\frac{u_{e,s}}{u_{mf}}\right)^{0.7} = \left(\frac{\varepsilon_e(1-f_b)u_e}{u_{mf}}\right)^{0.7} \quad (101)$$

$$\left(\frac{1-\varepsilon_{mf}}{1-\varepsilon_e}\right) = \frac{2.54\rho_g^{0.016}\mu^{0.066}\exp(0.090P_{45\mu m})}{d_p^{0.1}g^{0.118}(\rho_s-\rho_g)^{0.118}H_{mf}^{0.043}} \quad (102)$$

For larger Geldart B and D type particles, Hillgardt and Werther [1986] found that the amount of gas that actually passes through the emulsion phase can be significantly higher than u_{mf} , with only 1/3 (3D beds) or 1/8 (2D beds) of the gas in excess of u_{mf} going to the bubble phase.

Effective diffusivity in the emulsion phase:

From energy dissipation studies, Baird and Rice [1975] correlated the effective diffusivity in the emulsion phase as follows:

$$D_e = 0.35(gu_s)^{1/3}d_t^{4/3} \quad (103)$$

The correlation was, however, derived for a variety of bubble flows and specifically for the fluidized bed data, the fit between the experimentally measured and predicted values was relatively poor.

Furthermore, data for small-diameter beds ($d_t < 7.6$ cm) were not included in the analysis. From experiments with small-diameter beds, Mireur and Bischoff [1967] derived a correlation that typically gives smaller values of D_e :

$$D_e = \frac{u_s Z^{2.5}}{0.33 d_t^{1.5}} \quad (104)$$

valid over a wide range of u_s/u_{mf} .

Effective thermal conductivity in the radial direction and convective heat transfer coefficient in the vicinity of the wall:

Wender and Cooper [1958] correlated the Nusselt number for heat transfer between the bed and the reactor or tube wall as a function of the particle Reynolds number based on data obtained from different fluidized beds as shown in Figure 5. Levenspiel and Walton [1954] proposed from experiments in a 10.3 cm diameter bed with air and with glass and coal particles with $d_p = 0.15 - 4.34 \text{ mm}$:

$$\frac{\alpha_w d_p}{\lambda_f} = 0.6 \text{ Pr } \text{Re}_p^{0.3} \quad (105)$$

Alternative correlations were proposed by Van Heerden et al. [1953], Dow and Jacob [1951] and Toomey and Johnstone [1953]. Wen and Leva [1956] correlated the data of these authors combined with their own data [Oka, 1994].

Specific correlations for the effective thermal conductivity in the radial direction, λ_{er} , are challenging to measure because, due to the efficient mixing of the particle bed, heat transfer between the reactor wall and the bed is typically assumed to be limited by heat transfer in the near-wall region. A distinction can be made between large particles with a short contact time with the wall and small particles contacting the wall within a packet of particles leading to long contact times. With large particles and short contact times, heat transfer in the first layer of particles in direct contact with the wall has to be considered, whereas thermal diffusion into the rest of an emulsion packet can be neglected. A correlation derived by Glicksman and Deckers [1983] from experimental data ($1 \text{ mm} < d_p < 4 \text{ mm}$, $P = 1-10 \text{ atm}$, $\text{Re}_p = 10 - 3,500$) is reported in Kunii and Levenspiel [1991] for such cases:

$$\frac{\alpha_w d_p}{\lambda_f} = (1 - f_b)(5.0 + 0.05 \text{ Pr } \text{Re}_p) \quad (106)$$

In the case of small (Geldart A type) particles exposed to prolonged contact with the wall as they reside in an emulsion packet, thermal diffusion in the emulsion packet becomes heat transfer limiting. Starting from a surface renewal model, Mickley and Fairbanks [1955; 1961] proposed a correlation for the instantaneous heat transfer coefficient. A time-averaged heat transfer coefficient then follows from an integration over possible contact times [Kunii and Levenspiel, 1991]:

$$\alpha_{w,packet} = 1.13 \left[\frac{\lambda_b^0 \rho_s (1 - \varepsilon_{mf}) c_{p,s} n_w}{1 - f_{b,w}} \right]^{1/2} \quad (107)$$

Information on the static contribution of the thermal conductivity in a fixed bed, λ_b^0 , can be found in Froment et al. [2010]. Correlations for the fraction bubbles in the reactor in the near-wall region, $f_{b,w}$, or for the bubble frequency in the near-wall region, n_w , are challenging to find. A correlation for the bubble frequency just above an orifice can be found in Kunii and Levenspiel [1991]:

$$n_b = \frac{54.8}{F_{g,or}^{1/5}} \quad (108)$$

for n_b in $[s^{-1}]$ and $F_{g,or}$ the volumetric flow rate of gas through an orifice in $[cm^3/s]$. The bubble frequency in the bed was in general observed to be a factor 2-3 lower than predicted by Eq. (107) as a result of the rapid formation of bubble doublets and triplets. Using the analogy with bubble formation in an inviscid liquid [Harrison and Leung, 1961], Davidson and Harrison [1963] derived a similar expression for the bubble frequency, assuming there is no gas leakage between bubble and emulsion phase:

$$n_b = \frac{21.7}{F_{g,or}^{1/5}} \quad (109)$$

using the same units as in Eq. (108) and indeed resulting in frequencies 2-3 times lower. Predictions were found satisfactory at high gas flow rates. At low gas flow rates, viscosity effects are important, and the inviscid liquid theory somewhat underestimates the bubble size and overestimates the bubble frequency. Based on the Davidson and Schuler [1960] equation for the bubble size [Yang, 2003]:

$$n_b = \frac{17.92}{F_{g,or}^{1/5}} \quad (110)$$

From experiments with two-plane ECT sensors in a 10.4 cm diameter, 1.4 m height column fitted with a porous plate distributor and using six different types of particles with mean particle diameter 180-2200 μm and particle density in the range 1,300-2,837 kg_s/m_s^3 , Agu et al. [2019] derived a correlation for the bubble frequency in bubbling fluidized beds:

$$n_b = \left[0.52 \left(\frac{d_b}{d_t} \right)^{1.48} + m u_b^n d_b \right]^{-1} \quad (111)$$

, where proper correlations for the bubble diameter, d_b , and the bubble velocity, u_b , are used and for the bubbling regime, $m = 0.05$ and $n = -3.475$ for Geldart A and $n = -4.379$ for Geldart B type particles.

Radiative heat transfer was found to contribute significantly with larger particles (e.g. Geldart D-type). With small (Geldart A type) particles, as typically used in kinetic studies, radiative heat transfer is about an order of magnitude less important than other heat transfer mechanisms [Oka, 1994]. For bed materials with emissivity of the particles $0.3 < \epsilon_p < 0.6$ [Baskakov, 1985]:

$$\alpha_{rad} = 7.3 \sigma \epsilon_p \epsilon_s T_s^3 \quad (112)$$

where ϵ_s is the emissivity of the heat exchange surface.

As the effective thermal conductivity in the bed is strongly related to the effective diffusion of the particles in the bed, λ_{er} can be estimated from [Oka, 1994]:

$$\lambda_{er} = D_{er} \rho_s c_{p,s} (1 - \epsilon) \quad (113)$$

The effective diffusivity in the radial direction is, however, about one order of magnitude smaller than the effective diffusivity in the axial direction, as calculated by Eqs. (103) or (104) [Oka, 1994].

Kunii and Levenspiel [1969] proposed the following correlation for the radial dispersion coefficient of the solids in the bed:

$$D_{er} = \frac{3}{16} \left(\frac{f_b}{1-f_b} \right) \frac{u_{mf} d_b}{\epsilon_{mf}} \quad (114)$$

An alternative correlation claiming to be more generally applicable was derived by Shi and Fan [1984] based on dimensional analysis and regression of literature data:

$$D_{er} = 0.46 (u_s - u_{mf}) Z_{mf} \left[\frac{(u_s - u_{mf}) d_p \rho_f}{\mu} \right]^{-0.21} \left[\frac{Z_{mf}}{d_p} \right]^{0.24} \left[\frac{\rho_s - \rho_f}{\rho_f} \right]^{-0.43} \quad (115)$$

Pillai [1981] carried out measurements with silica sand (255-425 μm) and silicon carbide particles (355-510 μm) at superficial gas velocities up to $6 \times u_{mf}$ and found that for these low solids' conductivity materials, the solids motion determines heat transfer with the tube wall. The data showed little influence of the particle size or particle density and a weak influence of the solids' conductivity. A linear relation between λ_{er} and the so-called fluidization index $(u_s - u_{mf})/u_{mf}$ was found:

$$\lambda_{er} = 0.03 + 0.05 \frac{(u_s - u_{mf})}{u_{mf}} \quad (116)$$

The data confirmed that with values of 0.03-0.33 kW/m/K, the effective thermal conductivity in the radial direction is an order of magnitude smaller than in the axial direction.

Interchange coefficient for mass transfer between the bubble phase and the emulsion phase:

Van Swaaij and Zuiderweg [1972] proposed:

$$k_I = \frac{u_s}{\left(1.8 - \frac{1.06}{d_t^{1/4}}\right) \left(3.5 - \frac{2.5}{Z^{1/4}}\right)} \quad (117)$$

Kunii and Levenspiel [1969; 1991] refined the model to account for presence of a cloud in between the bubble and emulsion phase, mass transfer becoming two steps in series, so that:

$$\frac{1}{(k_I)_b} = \frac{1}{(k_{bc})_b} + \frac{1}{(k_{ce})_b} \quad (118)$$

Correlations were proposed on a per m^3 bubble basis. Hence:

$$k_I = (k_I)_b f_b \quad (119)$$

For the coefficients $(k_{bc})_b$ and $(k_{ce})_b$:

$$(k_{bc})_b = 4.5 \frac{u_{mf}}{d_b} + 5.85 \left(\frac{D^{1/2} g^{1/4}}{d_b^{5/4}} \right) \quad (120)$$

$$(k_{ce})_b = 6.77 \left(\frac{\varepsilon_{mf} D_{ce} u_{br}}{d_b^3} \right)^{1/2} \approx 6.77 \left(\frac{\varepsilon_{mf} D u_{br}}{d_b^3} \right)^{1/2} \quad (121)$$

Experiments with fine particle systems showed that the effective diffusion coefficient of the gas in the emulsion phase introduced in Eq. (121), D_{ce} , can best be approximated by the gas diffusivity, D , [Kunii and Levenspiel, 1991].

Gas-solids heat transfer coefficient:

In general, the heat transfer coefficient can be expressed by means of a j -factor [Froment et al., 2010]:

$$h_f = j_H c_p G Pr^{-\frac{2}{3}} \quad (122)$$

A correlation for the j_H -factor was proposed by Balakrishnan and Pei [1975] based on experimental data with various oxides, d_p : 3.2 mm – 6.4 mm, ρ_s : 827 – 1,939 kg_s/m_s^3 (Geldart D-type):

$$j_H = 0.043 \left[\frac{d_p g (\rho_s - \rho_g) (1 - \varepsilon)^2}{u_s^2 \rho_g} \right]^{0.25} \quad (123)$$

, where u_s is the superficial gas velocity in the bed.

Gupta and Thodos [1963] proposed:

$$j_H = j_D = \frac{2.06}{\varepsilon (Re_p)^{0.575}} \quad (124)$$

for $90 \leq Re_p \leq 4,000$ and for $0.6 < Pr < 60$, where for $Re_p > 1,900$, $j_H = 1.05 j_D$.

Eq. (124) is equivalent to:

$$Nu_{fs} = \frac{h_f d_p}{\lambda_g} = \left(\frac{2.06}{\varepsilon} \right) (Re_p)^{0.425} Pr^{0.33} \quad (125)$$

Re-examining fluid-particle heat transfer in fixed and fluidized beds, Gupta et al. [1974] derived:

$$\varepsilon j_H = \frac{2.876}{Re_p} + \frac{0.3023}{(Re_p)^{0.35}} \quad (126)$$

Eq. (126) was found to correlate successfully data in the Re_p range of 10-10,000. Extrapolation should be done with care, especially at $Re_p < 10$, where j_H is seen to drop sharply using Eq. (126). For $10 \leq Re_p \leq 2,000$, a correlation similar to Eq. (124) is reported in the Perry [1984]:

$$j_H = j_D = \frac{0.4548}{\varepsilon (Re_p)^{0.4069}} \quad (127)$$

Alternative empirical correlations have been proposed by several groups. An extension of a correlation reported by Froment et al. [2010] to account for the dependence on the Prandtl-number as typically encountered in packed beds is:

$$Nu_{bed,fs} = \frac{h_f d_p}{\lambda_g} = 0.017(Re_p)^{1.21} Pr^{0.33} \quad (128)$$

, where no Re_p validity range is reported. A similar expression was reported by Kothari [1967] valid in the region of rapidly falling Nusselt number with particle Reynolds number [Kunii and Levenspiel, 1991], for $0.1 < Re_p < 100$:

$$Nu_{fs} = \frac{h_f d_p}{\lambda_g} = 0.03(Re_p)^{1.3} Pr^{0.33} \quad (129)$$

Eq. (129) is based on a fluidized bed in plug flow. According to Lee and Miller [2013], the particle Reynolds number, Re_p , in Eq. (129) should be calculated using the conditions in the emulsion region.

Baskakov et al. [1974] derived for fluidized beds of particles with $0.16 \text{ mm} \leq d_p \leq 4 \text{ mm}$:

$$Nu_{fs} = 0.009(Ar)^{0.5} Pr^{0.33} \quad (130)$$

, with Ar given by Eq. (58).

Gas-solids mass transfer coefficient:

A frequently used correlation for the calculation of the gas-solids mass transfer coefficient, k_g , is:

$$k_g = \frac{j_D G}{M_m c_{tot} y_{fA}} Sc^{-2/3} = \frac{j_D u_s}{y_{fA}} Sc^{-2/3} \quad (131)$$

where j_D represents the j -factor for mass transfer. Using the Chilton-Colburn analogy between heat and mass transfer, the correlations Eqs. (123)-(130) used for j_H can also be used for j_D . Using particles of size 0.248-2 mm, an alternative correlation for j_D was reported by Hsiung and Thodos [1977], valid for $1 < Re_p < 200$ and $0.3 < Re_{p,mf} < 2,000$:

$$j_D Re_p = 0.040 Re_{p,mf} + 2.12(Re_{p,mf})^{0.41} + \frac{0.62}{(Re_{p,mf})^{0.51}} \quad (132)$$

with: $Re_{p,mf} = u_{mf}\rho_f d_p/\mu$. Prins et al. [1985] found that the gas-solid mass transfer coefficient only depends on the minimum fluidization velocity, with no influence of the fluidization velocity, and that the data of Hsiung and Thodos [1977] could be well correlated by:

$$j_{D,mf} = \frac{1.61}{\varepsilon_{mf}(\widehat{Re}_{p,mf})^{0.64}} \quad (133)$$

for $0.3 < \widehat{Re}_{p,mf} < 80$ and with: $\widehat{Re}_{p,mf} = u_{mf}\rho_f d_p/[\mu(1 - \varepsilon_{mf})]$. Extensions of Eq. (132) have been studied by Prins et al. [1985]. It is, however, challenging to measure and model gas-solids mass transfer independent of bubble-emulsion phase mass transfer, which is often rate limiting.

Therefore, global gas-solids mass transfer coefficients for the bed have often been studied and correlated.

Davidson and Harrison [1963] proposed the following correlation for k_g in the bed:

$$k_g = \frac{f(\varepsilon)}{\varepsilon} u_s (Re_p)^{-0.6} Sc^{-2/3} \quad (134)$$

with:

$$f(\varepsilon) = (1 - \varepsilon)^{0.5} \quad \text{for small values of } \varepsilon \quad (135)$$

$$f(\varepsilon) = 0.66\varepsilon^{0.5} \quad \text{for large values of } \varepsilon \quad (136)$$

Gupta and Thodos [1963] proposed for $90 \leq Re_{p,mf} \leq 4,000$:

$$Sh_{fS} = \frac{k_g d_p}{D} = \left(\frac{2.06}{\varepsilon}\right) (Re_p)^{0.425} Sc^{0.33} \quad (137)$$

, which is equivalent to:

$$k_g = \frac{2.06}{\varepsilon} u_s (Re_p)^{-0.575} Sc^{-2/3} \quad (138)$$

and shows similarity with the well-known Frössling [1938] correlation:

$$Sh_{fS} = \frac{k_g d_p}{D} = 2.0 + 0.552(Re_p)^{0.5} Sc^{0.33} \quad (139)$$

which is strictly applicable for a single spherical particle. Scala [2007] found that a Frössling-type equation could well describe mass transfer around a freely moving active particle in the dense phase of a gas fluidized bed of inert particles.

Experiments with 1-10 mm active particles, 0.1-1.4 mm inert particles and fluidization velocities of 0.15-0.90 m/s showed that the Sherwood number is not influenced by the fluidization

velocity or fluidization regime, but increases with the square root of the minimum fluidization velocity and the active particle size. Scala [2007] proposed:

$$Sh_{fs} = \frac{k_g d_p}{D} = 2.0\varepsilon_{mf} + 0.7(Re_{p,mf}/\varepsilon_{mf})^{0.5} Sc^{0.33} \quad (140)$$

Studying air-solids systems ($Sc = 2.35$), correlations for particles of different size in terms of the Sherwood number of the bed were derived by Resnick and White [1949]. For the smallest particles studied, $d_p = 275 \mu m$, the following correlation was retrieved for Sh_{bed} for $4 < Re_p < 15$ [Yang, 2003]:

$$Sh_{bed} = \frac{k_g d_p}{D} = 0.041(Re_p)^{1.036} \quad (141)$$

Mass transfer between isolated active particles in a fluidized bed of inert particles and the fluidizing gas was studied by several groups – see reviews by Agarwal and La Nauze [1989] and Linjewile and Agarwal [1990]. Hsiung and Thodos [1977] and Kok et al. [1986], for example, measured the mass transfer coefficient using naphthalene particles in a bed of inert particles of about same size and density. The drying of moist particles in a fluidized bed of similar dry particles was also studied [Vandershuren and Delvossalle, 1980]. Palchonok et al. [1992] combined earlier work by Palchonok and Tamarin [1984] and Avedesian [1972] to propose the following correlation:

$$Sh_{act,bed} = \frac{k_g d_p}{D} = 2\varepsilon_{mf} + 0.117Ar^{0.39}Sc^{0.33} \quad (142)$$

with the Archimedes number, Ar , as defined in Eq. (58).

A model for gas-solid mass transfer in the bed that explicitly accounts for the correlations for bubble-emulsion phase mass transfer was proposed by Kunii and Levenspiel [1991].

ANNEX II. CRITERIA FOR NEGLIGIBLE RADIAL TEMPERATURE GRADIENTS

Criteria for negligible radial heat transport limitations in fluidized beds, as required for isothermal operation, can be derived in a similar way than those for fixed beds [Mears, 1971a; 1971b]. The criteria are based on comparing reaction rates in the bed and in the immediate vicinity of the wall and imposing a maximum allowable relative error on the observed reaction rate, Δr_{rel} , Eq. (51):

$$\frac{\bar{r}_A - r_{A,w}}{r_{A,w}} < \Delta r_{rel}$$

The criteria are derived starting from the steady state heat balance for the extreme case where there is no axial convection and focusing on the axial position where the cold or hot spot is located:

$$-\lambda_{er} \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) \Big|_{z=z_{hotspot}} = r_A \rho_B (-\Delta H) \quad (143)$$

An analytical solution was derived by Chambré and Grossman [1955]:

$$\theta - \theta_{max} = -2 \ln[B(r')^2 + 1] \quad (144)$$

with the dimensionless variables and parameters:

$$\theta = \frac{E(T - T_w)}{RT_w^2}$$

$$r' = \frac{r}{R_t}$$

$$B = \frac{\delta}{8} e^{|\theta_{max}|}$$

$$\delta = \frac{(-\Delta H) r_A(T_w) \rho_B R_t^2 E}{\lambda_{er} T_w^2 R}$$

where θ_{max} is the maximum dimensionless temperature. In the case where B and δ are sufficiently small, the logarithm can be approximated by its first order Taylor series around unity, so that:

$$\theta - \theta_{max} \cong -2B(r')^2 \quad (145)$$

The reaction rate is defined as:

$$r_A = A e^{\frac{-E}{RT}} f(C) \quad (146)$$

Considering the first order Taylor series around $r_A(T_w)$ gives:

$$r_A(T) = r_A(T_w) \left(1 + \frac{T - T_w}{T_w} \frac{E}{RT_w} \right) \quad (147)$$

Substituting Eq. (145) into Eq. (147), the average reaction rate in the cross section follows from:

$$\pi 1^2 \bar{r}_A = r_{A,w} \int_0^1 [1 + \theta_{max} - 2B(r')^2] 2\pi r' dr' \quad (148)$$

From the solution of Eqs. (143) / (148), the relative error on the reaction rate can be calculated so that criterion Eq. (51) becomes:

$$\frac{\bar{r}_A - r_{A,w}}{r_{A,w}} = \theta_{max} - B < \Delta r_{rel} \quad (149)$$

A first criterion is valid when the heat transfer resistance at the wall can be neglected, typically justified for $d_t/d_p > 100$. With negligible heat transfer resistance at the wall:

$$\theta = 0 \text{ for } r' = 1 \quad (150)$$

From Eq. (145) it then follows that:

$$\theta_{max} = 2B \quad (151)$$

From the definition of B and expanding the Taylor series of the exponential:

$$\theta_{max} = 2B = \frac{\delta}{4} e^{|\theta_{max}|} \cong \frac{\delta}{4} (1 + \theta_{max}) = \frac{\delta/4}{1 - \delta/4} \cong \frac{\delta}{4} \quad (152)$$

Substituting Eq. (152) in Eqs. (149) / (150) results in:

$$\frac{\delta}{4} - \frac{\delta}{8} e^{\frac{\delta}{4}} \approx \frac{\delta}{8} < \Delta r_{rel} \quad (153)$$

Accounting for the definition of δ then leads to Eq. (52):

$$\Delta T_{c,w} = \frac{|\Delta H| r_A(T_w) \rho_B d_t^2}{16 \lambda_{er}} < \Delta r_{rel} \frac{2RT_w^2}{E}$$

where $\Delta T_{c,w}$ represents the temperature difference between the centre of the bed and the inner wall (K).

The second criterion accounts for dominant heat transfer limitations in the near wall region and is typically applied $d_t/d_p < 100$. The boundary condition is then defined by:

$$-\lambda_{er} \left. \frac{\partial T}{\partial r} \right|_{r=R_t} = \alpha_w (T_{R_t} - T_w) \quad (154)$$

which can be written in dimensionless numbers as:

$$\left. \frac{\partial \theta}{\partial r'} \right|_{r'=1} = \frac{-\alpha_w R_t}{\lambda_{er}} \theta_{r'=1} = \frac{-Bi_w R_t}{2 r_p} \theta_{r'=1} = \frac{-\widetilde{Bi}_w}{d_t} \theta_{r'=1} \quad (155)$$

with $Bi_w = \alpha_w d_p / \lambda_{er}$ the particle diameter based Biot number and $\widetilde{Bi}_w = \alpha_w d_t / \lambda_{er}$ the tube diameter based Biot number. Considering θ_{max} is small to reduce the Taylor series of the exponential to unity:

$$\theta_{r'=1} = \theta_{max} - 2B = \theta_{max} - \frac{\delta}{4} \quad (156)$$

$$\left. \frac{\partial \theta}{\partial r'} \right|_{r'=1} = -4B = -\frac{\delta}{2} \quad (157)$$

Substituting Eqs. (156) and (157) in Eq. (155) results in:

$$-\frac{\delta}{2} = \frac{-Bi_w R_t}{2} \frac{R_t}{r_p} \left(\theta_{max} - \frac{\delta}{4} \right) = \frac{-\widetilde{Bi}_w}{2} \left(\theta_{max} - \frac{\delta}{4} \right) \quad (158)$$

or:

$$\theta_{max} = \frac{\delta}{4} + \frac{r_p}{Bi_w R_t} \delta = \frac{\delta}{4} \left(1 + \frac{4}{Bi_w} \frac{r_p}{R_t} \right) = \frac{\delta}{4} \left(1 + \frac{4}{\widetilde{Bi}_w} \right) \quad (159)$$

Criterion Eq. (149) can then be developed as:

$$\frac{\delta}{4} \left(1 + \frac{4}{Bi_w} \frac{r_p}{R_t} \right) - \frac{\delta}{8} e^{\frac{\delta}{4} \left(1 + \frac{4}{Bi_w} \frac{r_p}{R_t} \right)} \cong \frac{\delta}{8} \left(1 + \frac{8}{Bi_w} \frac{r_p}{R_t} \right) = \frac{\delta}{8} \left(1 + \frac{8}{\widetilde{Bi}_w} \right) < \Delta r_{rel} \quad (160)$$

The condition for a sufficiently small radial temperature gradient for narrow reactors then becomes

Eq. (53):

$$\Delta T_{c,w} = \left(1 + \frac{8}{Bi_w} \frac{r_p}{R_t} \right) \frac{|\Delta H| r_A(T_w) \rho_B d_t^2}{16 \lambda_{er}} < \Delta r_{rel} \frac{2RT_w^2}{E}$$

or Eq. (54):

$$\Delta T_{c,w} = \left(1 + \frac{8}{\widetilde{Bi}_w} \right) \frac{|\Delta H| r_A(T_w) \rho_B d_t^2}{16 \lambda_{er}} < \Delta r_{rel} \frac{2RT_w^2}{E}$$

ANNEX III. CRITERIA FOR NEGLIGIBLE GAS-SOLID HEAT AND MASS TRANSFER LIMITATIONS

Negligible gas-solid heat transfer limitations:

The development of the criterion of Mears [1971a; 1971b] starts from the exponential dependence of the reaction rates on the temperature, $r_A(T) = k_0 e^{[-E/(RT)]} \times f(C_A)$. Taylor series expansion of the exponential function around the bulk temperature results in the following expression for the reaction rate at the solid surface temperature:

$$r_A(T_S) = r_A(T_B) \left(1 + \frac{T_S - T_B}{T_B} \frac{E}{RT_B} \right) \quad (161)$$

The criterion is based on a maximum allowable relative error on the measured reaction rate:

$$\frac{r_A(T_S) - r_A(T_B)}{r_A(T_B)} = \frac{T_S - T_B}{T_B} \frac{E}{RT_B} < \Delta r_{rel} \quad (162)$$

Considering the extreme case where no heat is evacuated or supplied by the flow of the particles itself, the local heat balance can be written:

$$(-\Delta H)r_A\rho_s\frac{4\pi}{3}\left(\frac{d_p}{2}\right)^3 = h_f(T_S^s - T_B)4\pi\left(\frac{d_p}{2}\right)^2 \quad (163)$$

so that:

$$(T_S^s - T_B) = \frac{(-\Delta H)r_A\rho_s d_p}{6h_f} \quad (164)$$

Substitution of Eq. (164) into Eq. (162) yields Eq. (78):

$$\Delta T_{s,f} = \frac{(-\Delta H)r_A\rho_s d_p}{6h_f} < \Delta r_{rel} \frac{RT_B^2}{E}$$

where $\Delta T_{s,f}$ is the temperature difference between the solid surface and the bulk fluid (K). The reaction rate, r_A , can be calculated with the bulk concentration, C_{AB} , and bulk temperature, T_B , assuming absence of gas-solid mass and heat transfer limitations and bubble-emulsion phase transport limitations.

Negligible gas-solid mass transfer limitations:

Identifying the relation between the reaction conditions – at the locus of reaction – and the reaction rates also requires negligible gas-solid mass transfer limitations. The derivation is similar to the one presented by Mears [1971a; 1971b] for fixed bed reactors. Expressing the rate of reaction as:

$$r_A = k \times f(C_A) \quad \text{with:} \quad f(C_A) = C_A^n \quad (165)$$

, the reaction rate at the solid surface can be developed as a first-order Taylor series around the concentration in the emulsion gas:

$$r_A(C_{A,s}^s) = r_A(C_{A,e}) \left(1 + n \frac{C_{A,s}^s - C_{A,e}}{C_{A,e}} \right) \quad (166)$$

The criterion is based on a maximum relative error on the measured reaction rate:

$$\frac{r_A(C_{A,e}) - r_A(C_{A,s}^s)}{r_A(C_{A,e})} = n \frac{C_{A,e} - C_{A,s}^s}{C_{A,e}} < RI_{im,r} \quad (167)$$

Considering the worst case where no species are supplied or evacuated by the flow of particles itself, a local species mass balance can be written similar to Eq. (163):

$$r_A \rho_s = k_g \frac{6}{d_p} (C_{A,e} - C_{A,s}^s) \quad (168)$$

so that:

$$(C_{A,e} - C_{A,s}^s) = \frac{r_A \rho_s d_p}{6k_g} \quad (169)$$

Substituting Eq. (169) into Eq. (167) leads to criterion Eq. (79):

$$\Delta C_{A,es} \approx \Delta C_{A,fs} = \frac{r_A \rho_s d_p}{6k_g} < RI_{im,r} \frac{C_{A,e}}{n}$$

where $\Delta C_{A,es}$ is the concentration difference between the emulsion fluid and the solid surface and $\Delta C_{A,fs}$ is the concentration difference between the bulk fluid and the solid surface. The reaction rate, r_A , can be calculated with the bulk concentration, C_{AB} , and bulk temperature, T_B , assuming absence of gas-solid mass and heat transfer limitations and bubble-emulsion phase transport limitations.

ANNEX IV. CRITERIA FOR NEGLIGIBLE INTRA-PARTICLE HEAT AND SPECIES TRANSPORT

LIMITATIONS

Negligible intra-particle heat transport limitations:

A criterion for negligible intra-particle heat transport limitations is based on a maximum relative error on the measured reaction rate [Anderson, 1963; Mears, 1971a; 1971b]:

$$\frac{\bar{r}_A - r_A(T_s^s)}{r_A(T_s^s)} < \Delta r_{rel} \quad (170)$$

with \bar{r}_A , the average reaction rate in a particle, defined as:

$$\bar{r}_A = \frac{\int_{V_p} r_A dV}{V_p} \quad (171)$$

With a reaction rate as in Eq. (165), a first-order Taylor series development around T_s^s allows to approximate T_s as:

$$r_A(T_s) = r_A(T_s^s) \left(1 + \frac{T_s - T_s^s}{T_s^s} \frac{E}{RT_s^s} \right) \quad (172)$$

Using Eq. (172):

$$\int_{V_p} r_A dV = \int_{V_p} r_A(T_s^s) \left(1 + \frac{T_s - T_s^s}{T_s^s} \frac{E}{RT_s^s} \right) dV \quad (173)$$

Anderson [1963] assumed a temperature profile of the form:

$$T_s - T_s^s = \sigma \left(1 - \left(\frac{2r}{d_p} \right)^2 \right) \quad (174)$$

with $\sigma = T_{s,r=0} - T_s^s$ depending on the heat of reaction. Expressing the volume according to the radius and introducing Eq. (174) in Eq. (173):

$$\int_{V_p} r_A dV = r_A(T_s^s) \int_0^{r_p} 4\pi r^2 + \frac{E\sigma}{RT_s^{s2}} \left(4\pi r^2 - \frac{4\pi r^4}{r_p^2} \right) dr \quad (175)$$

$$\int_{V_p} r_A dV = r_A(T_s^s) \left(\frac{4\pi r_p^3}{3} + \frac{E\sigma}{RT_s^{s2}} \frac{8\pi r^3}{5} \right) = r_A(T_s^s) \frac{\pi d_p^3}{6} \left(1 + \frac{E\sigma}{RT_s^{s2}} \frac{2}{5} \right) \quad (176)$$

The average reaction rate Eq. (171) can then be written as:

$$\bar{r}_A = r_A(T_s^s) \left(1 + \frac{2E\sigma}{5RT_s^{s2}} \right) \quad (177)$$

Criterion Eq. (170) hence becomes:

$$\frac{\bar{r}_A - r_A(T_s^s)}{r_A(T_s^s)} = \frac{2E\sigma}{5RT_s^{s2}} < \Delta r_{rel} \quad (178)$$

To relate σ introduced in Eq. (174) to the heat of reaction, the heat balance over a particle can be considered:

$$(-\Delta H)\bar{r}_A \rho_s V_p = -\lambda_e S_p \left. \frac{dT_s}{dr} \right|_{d_p} = \lambda_e S_p \frac{4}{d_p} \sigma \quad (179)$$

so that:

$$\sigma = \frac{(-\Delta H)\bar{r}_A \rho_s d_p^2}{24\lambda_e} \quad (180)$$

Substituting Eq. (180) into Eq. (178), the criterion for negligible intra-particle heat transport limitations becomes Eq. (80):

$$\sigma = \Delta T_{c,s} = \frac{(-\Delta H)\bar{r}_A \rho_s d_p^2}{24\lambda_e} < \Delta r_{rel} \frac{5RT_s^{s2}}{2E}$$

where $\Delta T_{c,s}$ is the temperature difference between centre and the external surface of the particle.

Negligible intra-particle species transport limitations:

Weisz and Prater [1954] developed a criterion to evaluate negligible intra-particle species transport limitations. The criterion was originally developed for a slab of catalyst but extended to other

geometrical shapes. The effectiveness factor compares the average reaction rate over a particle, or measured reaction rate, \bar{r}_A , with the rate of reaction at the particle surface:

$$\eta = \frac{\bar{r}_A}{r_A(C_{A,s}^s)} = \frac{\frac{1}{W_c} \int r_A(C_{A,s}) dW_c}{r_A(C_{A,s}^s)} = \frac{D_{eA} \frac{dC_{A,s}(L)}{dy}}{L r_A(C_{A,s}^s) \rho_s} \quad (181)$$

with L the position at the solid external surface. The calculation of Eq. (181) requires solution of the species continuity equation inside the catalyst slab:

$$\frac{d}{dy} \left(D_{eA} \frac{dC_{A,s}}{dy} \right) = r_A \rho_s \quad (182)$$

with boundary conditions:

$$\frac{dC_{A,s}(0)}{dy} = 0 \quad \text{and} \quad C_{A,s}(L) = C_{A,s}^s \quad (183)$$

Using the definition of the molar flux:

$$D_{eA} \frac{dC_{A,s}(L)}{dy} = \left(2 \int_{C_{A,s}^0}^{C_{A,s}^s} D_{eA} r_A \rho_s dc' \right)^{1/2} \quad (184)$$

the effectiveness factor Eq. (181) can be written:

$$\eta = \frac{\sqrt{2}}{L r_A(C_{A,s}^s) \rho_s} \left(\int_{C_{A,s}^0}^{C_{A,s}^s} D_{eA} r_A \rho_s dc' \right)^{1/2} \quad (185)$$

The effectiveness factor can be expressed in terms of a generalized modulus ϕ and is inversely proportional to ϕ when the latter is large, that is, with strong diffusion limitations [Froment et al., 2010]. In such case, the species concentration at the centreline will approach the equilibrium concentration (or zero for irreversible reactions), so that:

$$\phi = \frac{r_A(C_{A,s}^s) \rho_s}{\sqrt{2} a_g \left(\int_{C_{A,s,eq}}^{C_{A,s}^s} D_{eA}(C'_{A,s}) r_A(C'_{A,s}) \rho_s dC'_{A,s} \right)^{1/2}} \quad (186)$$

where a_g is the surface to volume ratio, $1/L$ for a slab geometry. With a reaction rate of order n :

$$r_A(C_{A,s}) = k C_{A,s}^n \quad (187)$$

By definition of the effectiveness factor Eq. (181):

$$\bar{r}_A \rho_s = \eta k C_{A,s}^n \rho_s \quad (188)$$

And Eq. (186) becomes:

$$\phi = \frac{kC_{A,s}^n \rho_s}{\sqrt{2}a_g \left(\int_{C_{A,s,eq}}^{C_{A,s}^S} D_{eA}(C'_{A,s}) k C_{A,s}^n \rho_s dC'_{A,s} \right)^{1/2}} = \frac{\sqrt{k\rho_s} C_{A,s}^n}{\sqrt{2}a_g \left(\int_{C_{A,s,eq}}^{C_{A,s}^S} D_{eA}(C'_{A,s}) C_{A,s}^n dC'_{A,s} \right)^{1/2}} \quad (189)$$

Introducing the square of Eq. (189) into Eq. (188) leads to:

$$\bar{r}_A \rho_s = \frac{\eta \phi^2 2a_g^2}{C_{A,s}^n} \int_{C_{A,s,eq}}^{C_{A,s}^S} D_{eA}(C'_{A,s}) C_{A,s}^n dC'_{A,s} \quad (190)$$

The Weisz-Prater modulus is obtained by grouping all measurable quantities on the right hand side:

$$\Phi = \eta \phi^2 = \frac{\bar{r}_A \rho_s C_{A,s}^n}{2a_g^2 \int_{C_{A,s,eq}}^{C_{A,s}^S} D_{eA}(C'_{A,s}) C_{A,s}^n dC'_{A,s}} = \frac{(n+1) \bar{r}_A \rho_s}{2a_g^2 D_{eA} C_{A,s}^S} \quad (191)$$

Negligible intra-particle species transport limitations are then ensured provided that criteria Eqs. (81)

and (82) are respected:

$$\frac{(n+1) \bar{r}_A \rho_s}{2a_g^2 D_{eA} C_{A,s}^S} < 0.33 \quad \text{for } n = 0$$

$$\frac{(n+1) \bar{r}_A \rho_s}{2a_g^2 D_{eA} C_{A,s}^S} < 0.08 \quad \text{for } n \geq 0.5$$

ANNEX V. SUMMARY OF CRITERIA

Flow pattern	
Fluidization	$u_{mf} < u_s$ $u_{i,fl} - u_{i,p} < u_t$
Bed turnover time	$t_T = Z_{mf} \rho_s (1 - \varepsilon_{mf}) / J$ <p>with: $J = \rho_s (1 - \varepsilon_{mf}) (u_s - u_{mf}) Y(\beta_w + 0.38\beta_d)$</p> <p>or: $J = 0.67 \rho_s (1 - \varepsilon_{mf}) (u_s - u_{mf}) \left(\frac{1}{\phi_b} - 1 \right)$</p>
Slugging	<p>For a distributor: $\frac{0.54}{g^{1/5}} (u_s - u_{mf})^{2/5} < \frac{d_t}{(Z + 4\sqrt{A_0})^{4/5}}$</p>

	<p>For a porous plate: $0.00853[1 + 27.2(u_s - u_{mf})]^{1/3}$</p> $< \frac{d_t}{(1 + 6.84Z)^{1.21}}$ <p>or:</p> $u_{br} > u_{b,ms} \quad \text{AND} \quad Z > z_s$ <p>with: $u_{b,ms} = u_{mf} + 7 \cdot 10^{-4}(gd_t)^{1/2}$</p> <p>or: $u_{b,ms} = u_{mf} + 7 \cdot 10^{-2}(gd_t)^{1/2} + 1.6 \cdot 10^{-3}(60d_t^{0.175} - Z_{mf})^2$</p> <p>and: $z_s = 60d_t^{0.175}$</p>
Channelling	$\Delta p_d \geq (0.2 - 0.4)\Delta p_b$ <p>or: $\Delta p_d \geq \Delta p_b \quad (Z < 0.3 \text{ m})$</p> <p>or:</p> $\frac{\Delta p_d}{\Delta p_b} \geq \left(\frac{L_f}{L_{mf}} - 1 \right) \frac{1}{1 - (u_{mf}/u_s)^n}$ <p>or:</p> $A_o < 0.1$
Axial dispersion	
Bubble phase	$Pe'_{a,b} = \frac{f_b^{3.56} Z}{56.4d_t^{1.33}(u_s - u_{mf})^{2.56}} \gg 1$ <p>or:</p> $Pe'_{a,b} = \frac{Z}{110d_t^2 u_{br}} \gg 1$
Emulsion gas	<p>Plug flow if: $Pe_{a,eg} = \frac{d_p u_e}{D_e} \gg \frac{\rho_e(1 - f_b)r_{A0}d_p}{u_e f_e C_{A0}}$</p> <p>CSTR if: $\left \frac{2 \left((1 + a)e^{\frac{a}{\gamma}} - (1 - a) - 2ae^{\frac{1}{2\gamma}} \right)}{(1 + a)^2 e^{\frac{a}{\gamma}} - (1 - a)^2 - 4ae^{\frac{(1+a)}{2\gamma}}} \right < \Delta r_{rel}$</p>

Isobaric operation	
Pressure drop over the bed	$L_{mf}(1 - \varepsilon_{mf})(\rho_s - \rho_g)g < 0.2 \frac{p_t}{n}$
Isothermal operation	
Radial temperature uniformity	<p>For $\frac{d_t}{d_p} > 100$: $\Delta T_{c,w} = \frac{ \Delta H r_A(T_w) \rho_B d_t^2}{16 \lambda_{er}} < \Delta r_{rel} \frac{2RT_w^2}{E}$</p> <p>For $\frac{d_t}{d_p} < 100$: $\Delta T_{c,w} = \left(1 + \frac{8}{Bi_w} \frac{r_p}{R_t}\right) \frac{ \Delta H r_A(T_w) \rho_B d_t^2}{16 \lambda_{er}} < \Delta r_{rel} \frac{2RT_w^2}{E}$</p>
Bed dilution & segregation	$\text{Segregation tendency} \propto [u_s - (u_{mf})_F] \left[\frac{(\rho_s)_J}{(\rho_s)_F} \right]^{-2.5} \left[\frac{(d_p)_B}{(d_p)_S} \right]^{-0.2}$
Adiabatic temperature rise	$\Delta T_{ad} = \frac{ \Delta H y_A^0 x_A}{c_{p,f} M_m}$
Interfacial transfer	
Bubble-emulsion mass transfer	<p>Plug flow emulsion gas: $\frac{nr_A(C_{A0})\rho_e(1 - f_b)}{2k_l C_{A0}} < RI_{im,r}$</p> <p>CSTR emulsion gas: $\left \frac{-nr_A(\bar{C}_A)\rho_e(1 - f_b)}{2k_l \left[C_{A0} - r_A(\bar{C}_A) \frac{\rho_e(1 - f_b)Z}{f_b u_b + f_e u_e} \right]} \right < RI_{im,r}$</p>
Gas-solid heat transfer	$\Delta T_{s,f} = \frac{ \Delta H r_A \rho_s d_p}{6h_f} < \Delta r_{rel} \frac{RT_B^2}{E}$
Gas-solid mass transfer	$\Delta C_{A,fs} = \frac{r_A \rho_s d_p}{6k_g} < RI_{im,r} \frac{C_{A,e}}{n}$

Intra-particle transport	
Intra-particle heat transfer	$\Delta T_{c,s} = \frac{(-\Delta H)\bar{r}_A \rho_s d_p^2}{24\lambda_e} < \Delta r_{rel} \frac{5RT_s^2}{2E}$
Intra-particle species diffusion	$\frac{(n+1)\bar{r}_A \rho_s}{2a_g^2 D_{eA} C_{A,s}^s} < 0.33 \quad \text{for } n = 0$ $\frac{(n+1)\bar{r}_A \rho_s}{2a_g^2 D_{eA} C_{A,s}^s} < 0.08 \quad \text{for } n \geq 0.5$