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TOWARDS A SINGLE EMPIRICAL CORRELATION TO PREDICT k_La ACROSS SCALES AND PROCESSES

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Introduction. Fermentation processes for the production of industrial enzymes are under continuous optimization so that the enzymes can be produced with a lower cost. Manipulation of media composition, strain improvements and various parameter optimizations (pH, temperature, etc.) are among the most relevant strategies for promoting the overproduction of bulk enzymes. Nevertheless, continued efforts towards finding further process improvements are needed if enzyme cost has to be reduced to make some processes economically feasible, or to stay competitive on a global market. One of the supporting tools that is increasingly used in the search for such improvements is the adaptation/formulation of mathematical models. However, one of the major limitations of these models relies in the fact that the parameters they include are often strain and scale dependent, meaning that they have to be determined every time a new process is introduced. The latter is obviously time consuming and not a trivial task. One of these parameters in aerobic fermentations is the volumetric mass transfer coefficient (k_La).
In this work, the oxygen transfer in different fermentation processes and at different scales will be study in order to establish a single equation to predict k_La.

Methodology. Operation data from a wide range of processes were extracted from the Novozymes pilot and production scale databases. On-line viscosity was measured for all processes, and a data set of 56 batches was produced. Numerical methods to deal with these large amount of data were developed. Off-line rheological measurements were performed for the pilot scale processes, 26 batches. The apparent viscosity was evaluated with 5 different calculations of the average shear rate in the tank, Table 1. The experimental k_La value was determined with the direct method; however, eight variations of the volumetric mass transfer coefficient calculation were evaluated taking into consideration different uncertainties around its estimation. Several simple correlations were formulated and were fitted by the least squares method to the eight measured k_La data set, along with the standard empirical correlation and some variations of it. For the on-line viscosity set, 18 correlations were fitted to the data, while 4 equations were tested for the off-line viscosity data set.

Table 1. Equations used to estimate the average shear rate in the tank to calculate the apparent viscosity.

Equation	Ref.
$\dot{\gamma} = k_s N$	(1)
$\dot{\gamma} = k_s N \frac{4n_{PL}}{(3n_{PL}+1)}^{n_{PL}/(1-n_{PL})}$	(2)
$\dot{\gamma} = \left(\frac{P}{V}\frac{1}{\mu_{app}}\right)^{1/2} \quad H/T = 1$	(3)
$\dot{\gamma} = \left(\frac{P}{V}\frac{1}{\mu_{app}}\right)^{1/2} \quad H/T \neq 1$	(3)
$\dot{\gamma} = \left(\frac{4P_0\,\rho D^5}{\pi H T^2\,K_{PL}}\right)^{1/(1+n_{PL})} N^{3/(1+n_{PL})}$	(4)

Results. The standard empirical equation was found to be the best correlation for predicting k_La in all processes in Novozymes fermentation pilot plant using off-line viscosity measurements. It was also found that the best method to estimate the shear rate corresponds to the equation developed based on dimensional analysis by Henzler and Kauling (3). In addition, a parameter set of the standard empirical equation was found that can predict oxygen transfer in low viscosity processes at all scales using on-line viscosity measurements.

Conclusions. Two sets of parameters to predict k_La based on the standard empirical equations for all processes - pilot scale and all scales - one process were found. However, no single correlation for all processes and all scales could be established.

Nomenclature.

D	Impeller diameter (m)
H	Un-gassed broth height (m)
K_{PL}	Consistency index (Pa $s^{n_{PL}}$)
k_s	Metzner & Otto constant (-)
N	Agitation speed (1/s)
n_{PL}	Flow behavior index (-)
P	Power draw (kW)
P_0	Un-gassed power number (-)
T	Tank diameter (m)
V	Volume broth (m^3)
$\dot{\gamma}$	Shear rate (1/s)
μ_{app}	Apparent viscosity (Pa s)

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