Extended photo-anaerobic model ePanM

In the volume of fluid model, the volume fraction of water is represented by the phase-field variable α. This way, values α = 1 and α = 0 correspond to cells entirely occupied by water and gas respectively. This phase field variable is used to confine the state variables and the source terms (e.g. reactions) to the water or gas phases. For simplification purposes, the gas phase will be represented by the symbol ψ = 1 – α. This way, the transport equations for the state variables are:

For variables whose transport is restricted to the water (A) and the gas phases (B) respectively.

This way, an A equation is solved for the variables SIC, SH2, SIN, XPB, XC, SHCO3, SNH3 and SH2PO4, whereas a B equation applies to the [H2]g and the [CO2]g equations. The ePanM model is run on a steady state bubble and velocity distribution. This is equivalent to the assumption that the time required for the bubbles to rise from the inlet to the headspace is negligible with respect to the time that would take to the gas concentration inside the bubbles to decrease significantly. Hence, the B equations are, in principle, not necessary.

In order to confine each variable to its corresponding phase, is to use the two scalar model. Each

For example, hydrogen can be present in the gas phase as H2, and in the liquid phase as dissolved hydrogen. These will be named, respectively , which exists only in the regions where , and , which exists only in the regions where . This must be taken into account in the description of the mass transfer/solubilization across the interface. For example, for the aforementioned hydrogen, it would be written as:

Where Aint is the gas/liquid interface area, is the mass transfer coefficient and is concentration of soluble hydrogen in the liquid phase if the latter was saturated and it is also a function of the local concentration of :

This means that, gas transfer across the interface can only occur in a volume element if these conditions are simultaneously met:

* The interface area is non-zero, which requires the volume element to contain both gas and liquid.
* is different than

For example, in the bulk of the gas phase the partial pressure of hydrogen is high, which in principle means that and , leading to solubilization of the gas in the liquid. Nevertheless, in the gas phase, the presence of liquid, hence the interface area is either 0 or negligible, which would result in a negligible transfer rate. The transfer/solubilization of CO2 gas in the liquid phase, or mathematically speaking, the conversion of into SC can be written in an analogous way. The other variables, are completely confined to one of the phases, hence it is sufficient to multiply the variable by the volume fraction of the phase they are confined to in their source terms. For example, the disappearance of purple phototropic bacteria is given by:

Which banishes along with Ψ, becoming 0 in the bulk of the gas phase. The following are a definition of the source terms. For simplification purposes, the tilde has been omitted, which means that the varaibles are already multiplied by the respective volume fraction, for example, in the definition of IIN, .

Limiting function for SIN

Limiting function for SIP

???

Soluble ions ??

reaction 1 (??)

disappearance of PPB

solubilization of hydrogen

solubilization of hydrogen

process A carbon ??

process A nitrogen ??

process A phosphorous ??

The set of transport equations conforming the ePanM model is the following: