WATER RESEARCH 60 (2014) 141–155

Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/watres

New systematic methodology for incorporating dynamic heat transfer modelling in multi-phase biochemical reactors

T. Fernández-Arévalo[*], *I. Lizarralde, P. Grau, E. Ayesa*

CEIT and Tecnun (University of Navarra), 15 Paseo Manuel de Lardizabal, San Sebastián 20018, Spain

ARTICLE INFO

Article history:
Received 17 September 2013
Received in revised form
17 January 2014
Accepted 18 April 2014
Available online 6 May 2014

Keywords:
Heat balance
Hess's law
Mathematical modelling
Multi-phase models
Plant-Wide Modelling methodology

ABSTRACT

This paper presents a new modelling methodology for dynamically predicting the heat produced or consumed in the transformations of any biological reactor using Hess's law. Starting from a complete description of model components stoichiometry and formation enthalpies, the proposed modelling methodology has integrated successfully the simultaneous calculation of both the conventional mass balances and the enthalpy change of reaction in an expandable multi-phase matrix structure, which facilitates a detailed prediction of the main heat fluxes in the biochemical reactors. The methodology has been implemented in a plant-wide modelling methodology in order to facilitate the dynamic description of mass and heat throughout the plant. After validation with literature data, as illustrative examples of the capability of the methodology, two case studies have been described. In the first one, a predenitrification-nitrification dynamic process has been analysed, with the aim of demonstrating the easy integration of the methodology in any system. In the second case study, the simulation of a thermal model for an ATAD has shown the potential of the proposed methodology for analysing the effect of ventilation and influent characterization.

1. Introduction

Operating temperature plays an important role in wastewater treatment efficiency (Metcalf and Eddy, 2004). Temperature dynamics affect microbial activity as well as physicochemical properties, such as dissolved oxygen saturation concentration, diffusivity, viscosity, density and the settling velocity (Sedory and Stenstrom, 1995). An increased temperature of a few degrees might stimulate the metabolic activity of the bacteria, while a substantial reduction of several degrees would result in reduced process stability, albeit temporarily, and a possible shift in the population of the reactor (Gallert and Winter, 2005). The causes of these temperature variations are often due to a combination of different factors. The most representative are conduction/convection phenomena, short-wave and long-wave radiations, the heat transmitted by the actuators and, to a greater or lesser degree, the heat produced or consumed by biochemical, chemical or physicochemical transformations. The influence of each term in the system is varied and depends largely on the analysed process and climate of the place. In the activated sludge units, a

---

[*] *Corresponding author*. Tel.: +34 943212800.
E-mail addresses: tfernandez@ceit.es (T. Fernández-Arévalo), ilizarralde@ceit.es (I. Lizarralde), pgrau@ceit.es (P. Grau), eayesa@ceit.es (E. Ayesa).

http://dx.doi.org/10.1016/j.watres.2014.04.034
0043-1354/

Nomenclature

$A_{bubbles}$	Contact area between aqueous phase and 2nd gas phase (m^2)
A_g	1st gas phase surrounding area (m^2)
A_{tank}	Contact area between aqueous phase and 1st gas phase (m^2)
A_w	Aqueous phase surrounding area (m^2)
$\overline{Cp_i}$	Specific heat capacity of *i* gaseous phase components at constant pressure ($kJ\ gE^{-1}\ K^{-1}$)
C_{pw,H_2O}	Specific heat capacity of water at constant pressure ($kJ\ gH_2O^{-1}\ K^{-1}$)
$\tilde{E}_{i,j}$	*i* phase stoichiometric matrix for the transformations between *i* and *j* phase
g	Gravitational acceleration ($m\ s^{-2}$)
Gr	Grashof number
$\bar{h}_{i,ref}$	Reference enthalpy of the *i* gaseous phase components ($kJ\ gE^{-1}$)
h_{w,ref,H_2O}	Reference enthalpy of water ($kJ\ gH_2O^{-1}$)
H_{Act}	Enthalpy transmitted from the actuators ($kJ\ d^{-1}$)
H_{atm_rad}	Longwave atmospheric radiation flux ($kJ\ d^{-1}$)
$H_{Cond/Conv}$	Surface conduction and convection enthalpy flux ($kJ\ d^{-1}$)
$\overline{H}_{in}$	Input enthalpy ($kJ\ d^{-1}$)
$\overline{H}_{out}$	Output enthalpy ($kJ\ d^{-1}$)
H_{sol_rad}	Shortwave solar radiation flux ($kJ\ d^{-1}$)
H_T	Net heat exchange of the analysed phase ($kJ\ d^{-1}$)
H_{trans}	Heat released or absorbed by the transformations in the analysed phase ($kJ\ d^{-1}$)
$k_{sol,rad}$	Total energy incident on the surface ($kJ\ d^{-1}\ m^{-2}$)
k_{wls}	Heat conduction through walls and pipes coefficient ($kJ\ d^{-1}\ K^{-1}\ m^{-2}$)
$\overline{\dot{m}}_{i,in}$	Inlet *i* phase mass flux ($gE\ d^{-1}$)
$\overline{\dot{m}}_{i,j}$	Mass flux transport between *i and j* phases ($gE\ d^{-1}$)
$\overline{\dot{m}}_{i,out}$	Outlet *i* phase mass flux ($gE\ d^{-1}$)
$\overline{M}_i$	Mass vector for the components present in the *i* phase (gE)
$n_{phs,i}$	Constant exponent of the *Pr* and *Gr* numbers (aqueous and *i* gaseous phases conduction/convection)
NC	No. of components in the *i* phase
NT	No. of transformations in the *i* phase
P_m	Power supplied by the engines and aeration systems ($kJ\ d^{-1}$)
Pr	Prandtl number
T_{atm}	Atmospheric temperature (K)
T_i	*i* phase temperature (K)
$T_{i,in}$	*i* phase inflow temperature (K)
$\overline{T}_{i,ref}$	Temperature corresponding to the reference enthalpy of the *i* gaseous phase components (K)
$T_{w,ref,H2O}$	Temperature corresponding to the reference enthalpy of water (K)
$\overline{X}_i$	Mass fraction of the gaseous phase components ($gE_i\ gE_{phase}^{-1}$)

Greek Symbols

$\alpha_{phs,i}$	Correction factor for surfaces facing up (aqueous and i gaseous phases conduction/convection)
α_{rad}	Solar absorptivity
β_{air}	Atmospheric radiation factor
β_{phs}	Coefficient of volume expansion (K^{-1})
δ	Characteristic length (m)
Δh_f	Specific formation enthalpy ($kJ\ gE^{-1}$)
Δh_r	Specific reaction enthalpy ($kJ\ gE^{-1}$)
ΔH_r	Net reaction enthalpy ($kJ\ d^{-1}$)
ε_{atm}	Surface emissivity
η_m	Efficiency of engines/aeration systems
$\overline{\lambda}_i$	Thermal conductivity of the *i* gaseous phase components ($kJ\ d^{-1}\ K^{-1}\ m^{-1}$)
λ_{atm}	Surface reflectivity
μ_{g1}	Dynamic viscosity of the gaseous phase components ($kgE\ m^{-1}\ s^{-1}$)
$\nu_{i,j}$	Rate coefficient for component *i* on process *j* ($gE_i\ gE_{reference\ component}^{-1}$)
$\overline{\rho}_{i,j}$	Kinetic rate for the transformations between *i* and *j* phases ($gE_{removed\ component}\ d^{-1}$)
σ	Stefan Boltzman constant ($kJ\ d^{-1}\ m^{-2}\ K^{-4}$)
υ_{g1}	Kinematic viscosity of the gaseous phase components ($m^2\ s^{-1}$)

Superscripts

*	Absolute temperature (°C)
°	Standard state values (25 °C)

Subscripts

g	gaseous phase
g_1	1st gaseous phase
g_1	2nd gaseous phase
in	Input
k	No. of state variables in the water phase
m	No. of state variables in the 1st gaseous phase
n	No. of transformations in the water phase
out	Output
s	solid phase
z	No. of state variables in the 2nd gaseous phase
w	Aqueous phase

typical diurnal temperature difference between water inlet and outlet fluxes only varies between 0.5 and 1 °C (Makinia et al., 2005). However, in some parts of the world, treatment systems are subjected to significant winter cooling and summer heating. In some nontemperate zones for instance, the atmospheric diurnal air temperature variation can be considerable, ranging from 2 °C during the early morning to over 25 °C during mid-afternoon (Paul, 2013), affecting considerably to the water temperature. In membrane bioreactors, the temperature rise in the tank may be quite significant comparing with the activated sludge reactors because of the higher biological heat production. These reactors have a higher biomass concentration and bacterial activity, which implies a higher biological heat production due to the exothermicity of the oxidation, nitrification and denitrification reactions (Sethi et al., 2011). In sludge line processes, the effect of temperature has greater importance and practically all units work above atmospheric temperature. The