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A THEORETICAL INVESTIGATION OF OXIDATION EFFICIENCY OF A VOLATILE REMOVAL ASSEMBLY REACTOR UNDER MICROGRAVITY CONDITIONS

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Introduction

Volatile Removal Assembly (VRA) is a subsystem of the Closed Environment Life Support System (CELSS) installed in the International Space Station. It is used for removing contaminants (volatile organics) in the wastewater produced by the space station crews. The major contaminants are formic acid, ethanol, and propylene glycol. The VRA contains a slim packbed reactor (3.5 cm diameter and four 28 cm long tubes in series) to perform catalyst oxidation of wastewater at elevated pressure and temperature under microgravity conditions. In the reactor, the contaminants are burned with oxygen gas (O_2) to form water and carbon dioxide (CO_2) that dissolves in the water stream. Optimal design of the reactor requires a thorough understanding about how the reactor performs under microgravity conditions. The objective of this study was to develop a mathematical model to interpret experimental data obtained from normal and microgravity conditions, and to predict the performance of VRA reactor under microgravity conditions.

Catalyst oxidation kinetics and the total oxygen-water contact area control the efficiency of catalyst oxidation for mass transfer, which depends on oxygen gas holdup and distribution in the reactor. The process involves bubbly flow in porous media with chemical reactions in microgravity environment. This presents a unique problem in fluid dynamics that has not been studied. Guo *et al.* (2004) developed a mathematical model that predicts oxygen holdup in the VRA reactor. No mathematical model has been found in the literature that can be used to predict the efficiency of catalyst oxidation under microgravity conditions.

Mathematical Model

A mathematical model has been developed in this study to simulate the oxidation efficiency of the VRA reactor. The longitudinal distribution of the oxygen mass flow rate in the reactor can be expressed as follows (derivation of the model is available from the author):

$$\dot{M}_{O2} = \dot{M}_{O2-0} \; e^{-\frac{3r_{O2}\Psi_b}{r_b \rho_{O2} v_b} x} \tag{1}$$

where $\dot{M}_{O2}$ is oxygen mass flow rate at the point x-distance from the reactor inlet, $\dot{M}_{O2-0}$ is oxygen mass flow rate at the reactor inlet, r_{O2} is rate of oxidation per unit contact area between oxygen and water, Ψ_b is the average sphericity of oxygen bubbles (the ratio of bubble's shortest diameter to longest diameter), r_b is the average radius of bubbles, ρ_{O2} is the density of oxygen gas, and v_b is the average velocity of bubbles.

It is customary to use the term oxygen utilization (U_{O2}) in evaluation of VRA reactor performance. The expression for U_{O2} can be theoretically derived based on Eq. (1):

$$U_{O2} = 1 - R_{O2-L} = 1 - e^{-\frac{3r_{O2}\Psi_b}{r_b \rho_{O2} v_b} L} \tag{2}$$

where L is the length of the reactor and R_{O2-L} is the remaining oxygen at the outlet of the reactor. The oxygen mass consumption potential in the reaction is then expressed as:

$$\Delta M_{O2} = U_{O2} \dot{M}_{O2-0} \; t_w \tag{3}$$

where t_w is the residence time of water in the reactor. The water residence time can be calculated based water injection rate, reactor size, packbed porosity, and oxygen holdup in the reactor. Based on the molar equivalency in the oxidation, the amount of organics i removed in the reaction can be expressed as:

$$\Delta M_i = \frac{\Delta M_{O2} W_{mi}}{32 N_i} \tag{4}$$

where W_{mi} is the molecular weight of organics i, and N_i is molar number of oxygen utilization for each mole of organics i defined in the following oxidation reaction:

$$n_i \, [\text{organics}] + m_i \, O_2 \Rightarrow p_i \, CO_2 + q_i \, H_2O, \tag{5}$$
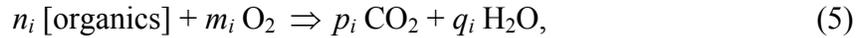
i.e., $N_i = m_i / n_i$. Typical values of N_i are shown in Table 1.

The oxygen mass flow rate at the reactor inlet $\dot{M}_{O2-0}$ is a design parameter. The density of oxygen gas (ρ_{O2}) can be calculated with gas law for ideal gas under given pressure and temperature. The sphericity of bubble (Ψ_b) may be affected by reactor geometry and gas holdup in the reactor. Due to lack of means of estimating its value, we used 0.5 throughout this study. The average flow velocity of oxygen bubbles (v_b) can be estimated based on oxygen injection rate, reactor cross-sectional area, packbed porosity, and oxygen holdup. The oxygen holdup can be estimated with the mathematical model described by Guo *et al.* (2004).

The rate of oxidation per unit water-oxygen contact area (r_{O2}) depends on the total flux rate (J) at which volatile organics disperse (Taylor, 1953):

$$J_i = -\left(\frac{D_{oi}}{F} + \frac{v_y^2 r_p^2}{48 D_{oi}} \right) \frac{dC_i}{dy} \tag{6}$$

where D_{oi} is the molecular diffusivity of organics i, F is called formation factor which is defined as tortuosity divided by porosity of packbed, $\frac{dC_i}{dy}$ is the concentration gradient of organics i in the direction perpendicular to the bubble surface, v_y is the average convection velocity, and r_p is the average pore radius.

A mathematical model was developed in this study to estimate the size of gas bubbles in a flowing liquid (derivation of the model is available from the author):

$$N_{WeC} = \frac{\rho_L d_m}{g \sigma} \left[1.1548 \sqrt{\frac{g d_m (\rho_L - \rho_g)}{\rho_L C_d}} - v_L \right]^2 \tag{7}$$

where N_{WeC} is the critical Weber number, ρ_L and ρ_g are densities of liquid and gas, respectively,

v_L is liquid velocity, and C_d is drag coefficient. If all other parameter values are known, the maximum bubble diameter d_m can be solved numerically from Eq. (7). The critical Weber number was determined to be 979 based on matching the calculated bubble diameter to the data (air bubble size in water). By matching the calculated oxygen bubble diameter to the observed oxygen bubble length (4 to 6 inches) under 1-G conditions, we estimated that the drag coefficient in the VRA reactor to be about $C_d = 3.9$.

Model Calibration

The VRA reactor performance data obtained from ethanol oxidation an experimental test conducted in ground surface conditions were used to calibrate the model. The reactor influent contained 144 mg/L of ethanol. The reactor effluent contained 91 mg/L of acetic acid and no ethanol. Material balance calculations show that the oxygen utilization is 87%. This value was obtained from the model by assuming that the organics concentrations drop from the initial concentrations in the pore space to zero at the catalyst surface within a distance of a half pore radius, and adjusting convection velocity to 0.2957 times the longitudinal water velocity.

Results

Figure 1 presents calculated oxygen mass flow rate under 1-G and 0.01-G conditions. In this case, the oxygen utilizations under 1-G and 0.01-G conditions are 63.42% and 60.11%, respectively. The calculated oxygen utilization drops by 5.23% under micro gravity conditions.

Conclusions

A mathematical model has been developed in this study to estimate oxidation efficiency in the VRA reactor under microgravity conditions. The following conclusions are drawn.

1. The remaining oxygen gas in the VRA reactor should decline exponentially with reactor length. The decline rate is directly proportional to rate of oxidation per unit area and bubble sphericity, and inversely proportional to bubble size, oxygen density and bubble velocity.

2. Gravity affects oxygen utilization through changing several parameters including oxygen bubble size. More research efforts are required to further investigate the effects of microgravity on VRA reactor performance.

3. The currently VRA design is very conservative. The oxygen utilization is about 60%.

Acknowledgements

References

[1] Guo, B., Holder, D.W., and Layne, C.: "Distribution of Flowing Fluids in a Confined Porous Medium under Microgravity Conditions," Physics of Fluids (August 2004), **16**, No. 8, 1-6.

[2] Taylor, G.I.: "Dispersion of Soluble Matter in Solvent Flowing Slowly though a Tube," Proc., Roy. Soc., **219** (1953), 186-194.

Table 1 – Baseline Concentration of Volatile Organics in the Waste Water

| Organics Name	Molecular Weight	Liquid Molecular Diffusivity (cm^2/s)	Molar Number of Oxygen Utilization	Influent Concentration (mg/L)
Acetaldehyde	44.05	0.00006953	2.5	2.74
Acetone	58.08	0.00005924	4	4.41
1-butanol	74.1	0.00005924	6	1.5
Ethanol	46.07	0.00006953	3	39.2
Ethylene glycol	62.07	0.00005924	2.5	5.51
Formaldehyde	30.03	0.00006953	1	5.89
Formic Acid	46.03	0.00006953	0.5	49.9
Methanol	32.04	0.00006953	1.5	7.94
Propylene glycol	76.1	0.00005924	4	35.4
1-propanol	60.1	0.00005924	4.5	0.45
2-propanol	60.1	0.00005924	4.5	1.6
Urea	60.06	0.00005924	1.5	3.55
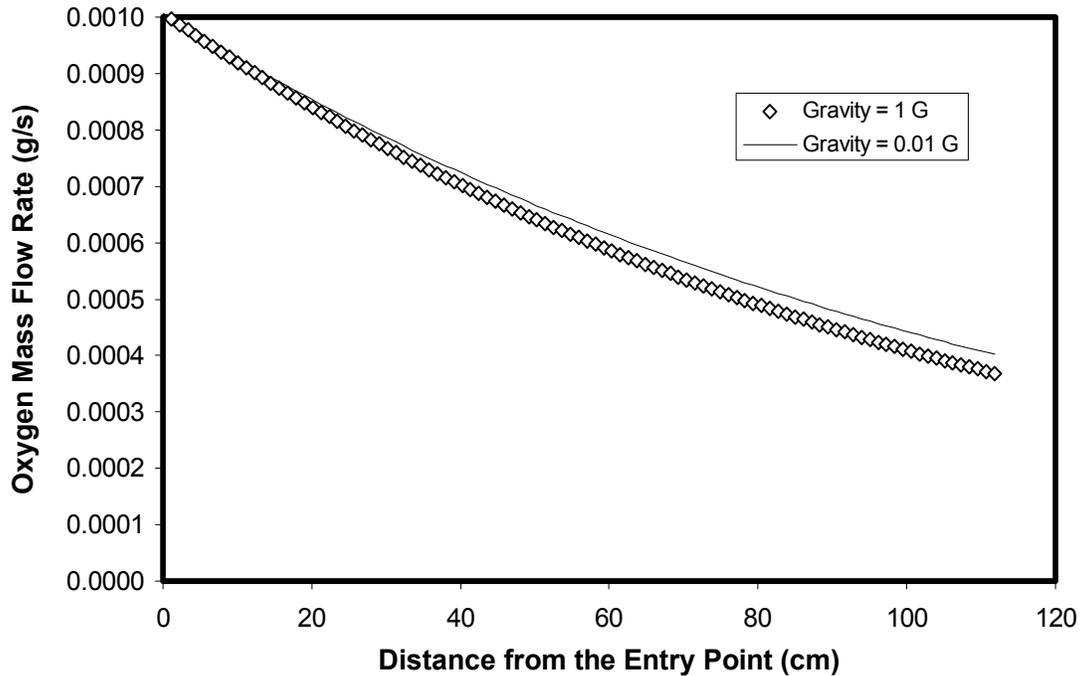
Figure 1 – Model-Calculated oxygen mass flow rate under 1-G and 0.01-G conditions