**Equations for Total Ion Criteria Development Ca Dependence**

**(Russell Erickson, 6/20/2023)**

**A. Model A**

*This simple linear model for log{TotIon} vs log{Ca} is unrealistic in not having lower/upper limits for the Ca dependence, but was included to evaluate whether a more complicated model was needed.*

(1) Basic Equation:



(2) Parameters:

(a) Slope – slope for log{X} vs log{Ca}

(b) logLC50XOnly@{Ca}=1 – intercept for log{X}, at log{Ca}=0

**B. Model B**

*This model maintains linearity of log{TotIon} vs log {Ca} at low Ca, but then transitions to an upper asymptote, using a formula of the form y=(1-e-x).*

(1) Basic Equation:



(2) Parameters:

(a) LC50XMax – hypothetical asymptote for LC50XOnly at high Ca

(b) {Ca}T – transition point between linear portion and asymptote

(c) Slope – limiting slope for log{X} vs log{Ca} at low Ca

(3) Because LC50XMax is not directly observed, model reparameterized to have LC50XOnly@{Ca}=1 as parameter instead. However, flattening can be at low enough Ca that this doesn’t have much effect.



**C. Model C**

*Due to indications of nonlinearity (increasing slope) at low Ca for Cerio, the following model was developed. It is assumed that the increasing slope is due to approaching a minimum Ca at which the organisms would not survive regardless of the elevation of other ions; i.e., there is an asymptote at this minimum Ca as well as the asymptote defining the maximum LC50XOnly at high Ca. This is described by a hyperbolic relationship on the log scale.*

(1) Basic Equation:



(2) Parameters:

(a) LC50XMax – hypothetical asymptote for LC50XOnly at high Ca

(b) {Ca}Min – asymptote at minimum tolerated Ca

(c) Sharp – sharpness of hyperbola

(3) This model also reparameterized with LC50XOnly@{Ca}=1.



**D. Model D**

*When linearity is desired at low Ca, Model B is complex to analyze and present. Therefore, a simpler model with linear log{TotIon} vs log {Ca} and asymptote for logLC50XOnly at high Ca was formulated, with the general form y=x/(x+k):*

(1) Basic Equation:



(2) Parameters:

(a) LC50XMax – hypothetical asymptote for LC50XOnly at high Ca

(b) {Ca}T – transition point between linear portion and asymptote

(c) Slope – limiting slope for log{X} vs log({Ca}/{Ca}T) at low Ca

(3) This model also reparameterized with LC50XOnly@{Ca}=1.



**E. Model E**

*This model also employs an exponential formula for an approach to an asymptote, but for log variables so of the form logY=(1-e-logX). This is not linear in log{X} vs log{Ca} (like Model B) nor is it asymptotic (like Model C) at low Ca. It was formulated to provide the possibility of more flattening at high Ca than Model C and less than Model B.*

(1) Basic Equation:



(2) Parameters:

(a) LC50XMax – asymptote for LC50XOnly at high Ca

(b) {Ca}T – transition point between steeper portion and asymptote

(c) Const (<1) – base for exponent affects shape/scale

(3) Because LC50XMax is not directly observed, model reparameterized to have LC50XOnly@{Ca}=1 as parameter instead. However, flattening can be at low enough Ca that this doesn’t have much effect.

