Analytical Integration Procedures for the Derivation of Risk Based Generic Assessment Criteria for Soil

Prof. Mengfang Chen

Institute of Soil Science
Chinese Academy of Sciences
Outline of the Presentation

◆ Brief History of CLEA Model Development
◆ Model Limitations
◆ Estimation of Human Exposure
◆ Analytical Integration Procedures
◆ Validation
◆ Summaries

M. Chen. Alternative integration procedures in combining multiple exposure routes for the derivation of generic assessment criteria with the CLEA model. *Land Contamination & Reclamation*, 18 (2), 2010

Brief History of CLEA Model Development

- **1992**: Start of the CLEA Development
- **1997**: CLEA 97 (CLR10)
- **2000**: Partial Probabilistic Approach
- **2002**: CLEA 2000 (CLR10)
- **2005**: CLEA UK (CLR10)
- **2006**: Deterministic Approach
- **2008**: CLAN 6/06
- **2009**: CLEA V1.03 beta(SR2)
- **2009**: CLEA V1.06
Model Limitations

- Vapour Saturation Limits NOT Considered
- Linear Relationship between ADE and Soil Concentration
- Leading to Unrealistic GAC (Not Capped by Soil Saturation Limits)
- Background Consideration – the 50% Rule
- Integration Methods
Model Limitations

Simplified versus Integrated Approach

\[ GAC = \min(GAC_{SS}, GAC_{ihm_{in}}, GAC_{ihm_{out}}) \]

\[ GAC_{int} \times \sum_{j=1}^{m} \sum_{o=1}^{n} R_{o}^{j} + \frac{GAC_{int} \times \sum_{j=1}^{f} \sum_{pv=1}^{n} R_{pv}^{j}}{TDI^{o} - ADE_{MDI}^{o}} + \frac{GAC_{int} \times \sum_{j=1}^{f} \sum_{pv=1}^{n} R_{pv}^{j}}{TDI^{i} - ADE_{MDI}^{i}} = 1 \]
**Model Limitations**

**Background Exposure: 50% Rule**

(a) Decreasing soil GAC as $ADE_{MDI}$ Increases

- $TDSI = TDI - ADE_{MDI}$
- $50\%$ Rule: $ADE_{MDI} = TDI/2$
- No Adjustment Required

(b) $ADE_{MDI}$ < $ADE_s$

- $50\%$ Rule Divide
- $ADE_{MDI}$

- $ADE_{MDI}$ ≥ $ADE_s$

- Adjustment Required: $ADE_{MDI}$ ≥ $ADE_s$

- $50\%$ Rule

- No Adjustment Required
Model Limitations

GAC/SGV Exceeding Soil Saturation Limits

- TDSI or ID
- GAC1 < \( C_{\text{SAT}} \)
- GAC2 > \( C_{\text{SAT}} \) under the linear partitioning
- GAC3 > \( C_{\text{SAT}} \) with the ADE capped for vapour pathways
- GAC3 > GAC2

ADE capped for Vapour Pathways
Estimation of Human Exposure

Calculation of Average Daily Exposure (ADE)

\[
A_{s}^{DE} = \sum_{j=1}^{t} \sum_{n=1}^{r} \frac{IR_{j}^{n} \times EF_{j}^{n} \times ED_{j}^{n}}{AT_{j}^{n} \times BW} = C_{S} \times \sum_{j=1}^{t} \sum_{o=1}^{m} R_{o}^{j} + C_{S} \times \sum_{j=1}^{t} \sum_{pv=1}^{n} R_{pv}^{j}
\]

Calculation of Background Exposure

\[
A_{MDI}^{o} = MDI^{o} \times \sum_{j=1}^{t} \frac{EF \times ED \times CF_{j}^{o}}{AT \times BW} \quad A_{MDI}^{i} = MDI^{i} \times \sum_{j=1}^{t} \frac{EF \times ED \times CF_{j}^{i}}{AT \times BW}
\]

Calculation of TOTAL Exposure

\[
A_{S+MDI}^{ADE} = A_{MDI}^{o} + A_{MDI}^{i} + GAC_{int} \times (\sum_{j=1}^{t} \sum_{o=1}^{m} R_{o}^{j} + \sum_{j=1}^{t} \sum_{pv=1}^{n} R_{pv}^{j})
\]
Estimation of Human Exposure

General Equation to Calculate Generic Assessment Criteria for Soil

\[
\frac{GAC_{\text{int}} \times \sum_{j=1}^{i} \sum_{o=1}^{m} R_{o}^{j}}{TDI^{o} - ADE_{MDI}^{o}} + \frac{GAC_{\text{int}} \times \sum_{j=1}^{t} \sum_{pv=1}^{n} R_{pv}^{j}}{TDI^{o} - ADE_{MDI}^{i}} = 1
\]
Estimation of Human Exposure

Equations to Calculate Generic Assessment Criteria for Soil

(Assumption: Oral TDI or Index Dose = Dermal TDI or Index)

Scenario 1: Oral $ADE_{MDI}^o > 50\%$ Oral TDI$^o$, Inhalation $ADE_{MDI}^i < 50\%$ Inhalation TDI$^i$

$$\frac{GAC_{int} \times \sum_{j=1}^t \sum_{o=1}^m R_o^j}{TDI^o - GAC_{int} \times \sum_{j=1}^t \sum_{o=1}^m R_o^j} + \frac{GAC_{int} \times \sum_{j=1}^t \sum_{p=1}^q R_p^j + c_{sat} \sum_{j=1}^t \sum_{v=1}^s R_v^j}{TDI^i - ADE_{MDI}^i} = 1$$

CLEA solution: the Goal Seek Function

AIP: Solution of a Polynomial Equation
Estimation of Human Exposure

Equations to Calculate Generic Assessment Criteria for Soil

(Assumption: Oral TDI or Index Dose = Dermal TDI or Index)

Scenario 2: Oral $ADE^o_{MDI} < 50\%$ oral TDI, Inhalation $ADE^i_{MDI} > 50\%$ Inhalation TDI

$$\frac{GAC_{int} \times \sum_{j=1}^t \sum_{o=1}^m R_{o}^j}{TDI^o - ADE^o_{MDI}} + \frac{GAC_{int} \times \sum_{j=1}^t \sum_{p=1}^q R_{p}^j + c_{sat} \sum_{j=1}^t \sum_{v=1}^s R_{v}^j}{TDI^i - (GAC_{int} \times \sum_{j=1}^t \sum_{p=1}^q R_{p}^j + c_{sat} \sum_{j=1}^t \sum_{v=1}^s R_{v}^j)} = 1$$

CLEA solution: the Goal Seek Function
AIP: Solution of a Polynomial Equation
Equations to Calculate Generic Assessment Criteria for Soil

(Assumption: Oral TDI or Index Dose = Dermal TDI or Index)

Scenario 3: Oral $ADE_{MDI}^o >50\%$ oral TDI$^o$, Inhalation $ADE_{MDI}^i >50\%$ Inhalation TDI$^i$

\[
\frac{GAC_{int} \times \sum_{j=1}^{t} \sum_{o=1}^{m} R^j_o}{TDI^o - GAC_{int} \times \sum_{j=1}^{t} \sum_{o=1}^{m} R^j_o} + \frac{GAC_{int} \times \sum_{j=1}^{t} \sum_{p=1}^{q} R^j_p + c_{sat} \sum_{j=1}^{t} \sum_{v=1}^{s} R^j_v}{TDI^i - (GAC_{int} \times \sum_{j=1}^{t} \sum_{p=1}^{q} R^j_p + c_{sat} \sum_{j=1}^{t} \sum_{v=1}^{s} R^j_v)} = 1
\]

CLEA solution: the Goal Seek Function

AIP: Solution of a Polynomial Equation
TABLE 6. Summary of Integration Procedures in Presence of NAPL

Solution to Equation 9b (outside the 50% Rule)

\[ GAC_{\text{sat}} = \frac{e-f-hc}{b+a(e-f)} \times (d-g) \]  \hspace{1cm} (13b)

Solution to Equation 10b (Limiting oral background exposure)

\[ GAC_{\text{sat}} = \frac{2ae-2af+db-ahc}{ab} - \sqrt{\left(\frac{2ae-2af+db-ahc}{ab}\right)^2 + \frac{2de-2ef-ahc}{ab}} \times \frac{2}{ab} \]  \hspace{1cm} (14b)

Solution to Equation 11b (Limiting inhalation background exposure)

\[ GAC_{\text{sat}} = \frac{2db+ae-ahc-2gb}{ab} - \sqrt{\left(\frac{2db+ae-ahc-2gb}{ab}\right)^2 + \frac{(d-g)(e-2hc)}{ab}} \times \frac{2}{ab} \]  \hspace{1cm} (15b)

Solution to Equation 12b (Limiting both oral and inhalation background exposure)

\[ GAC_{\text{sat}} = \frac{2db+2ae-3ahc}{3ab} - \sqrt{\left(\frac{2db+2ae-3ahc}{3ab}\right)^2 + \frac{(de-2dhc)}{3ab}} \times \frac{3}{3ab} \]  \hspace{1cm} (16b)
# HERA-Soil Model

## Validation

### TABLE 9. Comparison of the GAC<sub>int</sub> Derived from the CLEA and HERA-Soil model

<table>
<thead>
<tr>
<th>COC</th>
<th>Residential with Garden</th>
<th>Residential without Garden</th>
<th>Allotment</th>
<th>Commercial</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CLEA</td>
<td>HERA</td>
<td>CLEA</td>
<td>HERA</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>63.32</td>
<td>63.32</td>
<td>70.66</td>
<td>70.66</td>
</tr>
<tr>
<td>Xylene</td>
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<td>32.55</td>
<td>33.49</td>
<td>33.49</td>
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<tr>
<td>Naphthalene</td>
<td>8.71</td>
<td>8.71</td>
<td>9.22</td>
<td>9.22</td>
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<tr>
<td>Carbon Tetrachloride</td>
<td>0.089</td>
<td>0.089</td>
<td>0.0899</td>
<td>0.0899</td>
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<td>Cadmium</td>
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<td>30.16</td>
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<tr>
<td>Nickel</td>
<td>110.45</td>
<td>110.49</td>
<td>113.16</td>
<td>113.17</td>
</tr>
</tbody>
</table>

Note: unit: mg/kg
Summaries

- AIP accurately Solves GAC under the 50% Rule on the Background Exposure than the Goal Seek Function Implemented in the CLEA model.

- AIP providing additional functionalities of risk assessment models (Background Exposure, Vapour Saturation Limits)

- Reducing the speed of the simulation time if Applied within the CLEA model

- Improving GAC in less-sensitive land use (ie Commercial)

- To be implemented in an upcoming RA Model: SG-QRA_{dss}