ICCL
international
committee on
contaminated
land

October 4–5, 2011 ▪ Washington, DC Metro Area

10th Biennial Meeting

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

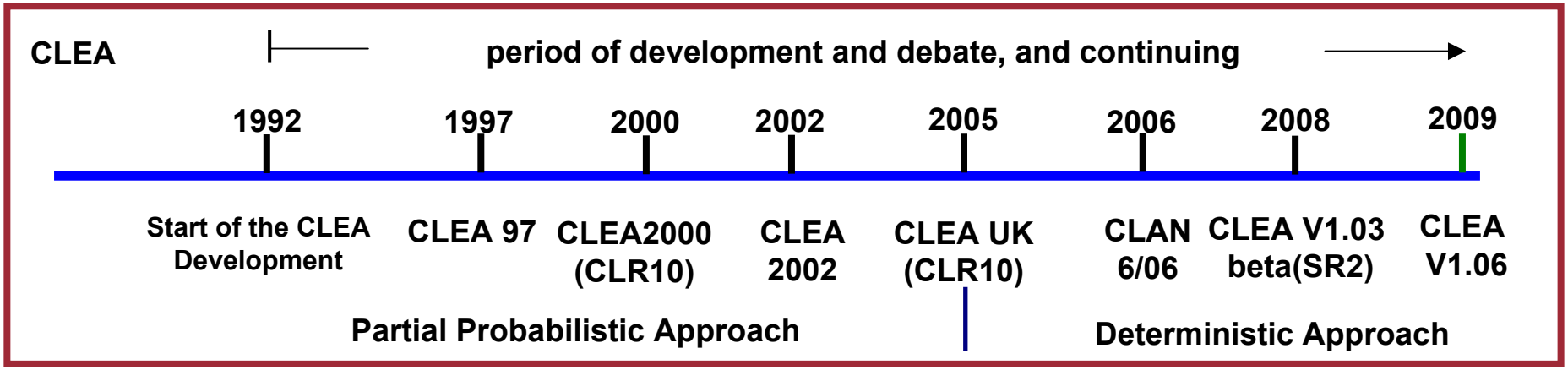
Outline of the Presentation

- 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

M. Chen. Analytical Integration Procedures for the Derivation of Risk-Based Generic Assessment Criteria for Soil**.** ***Human and Ecological Risk Assessment***, 16: 1295–1317, 2010

Brief History of CLEA Model Development

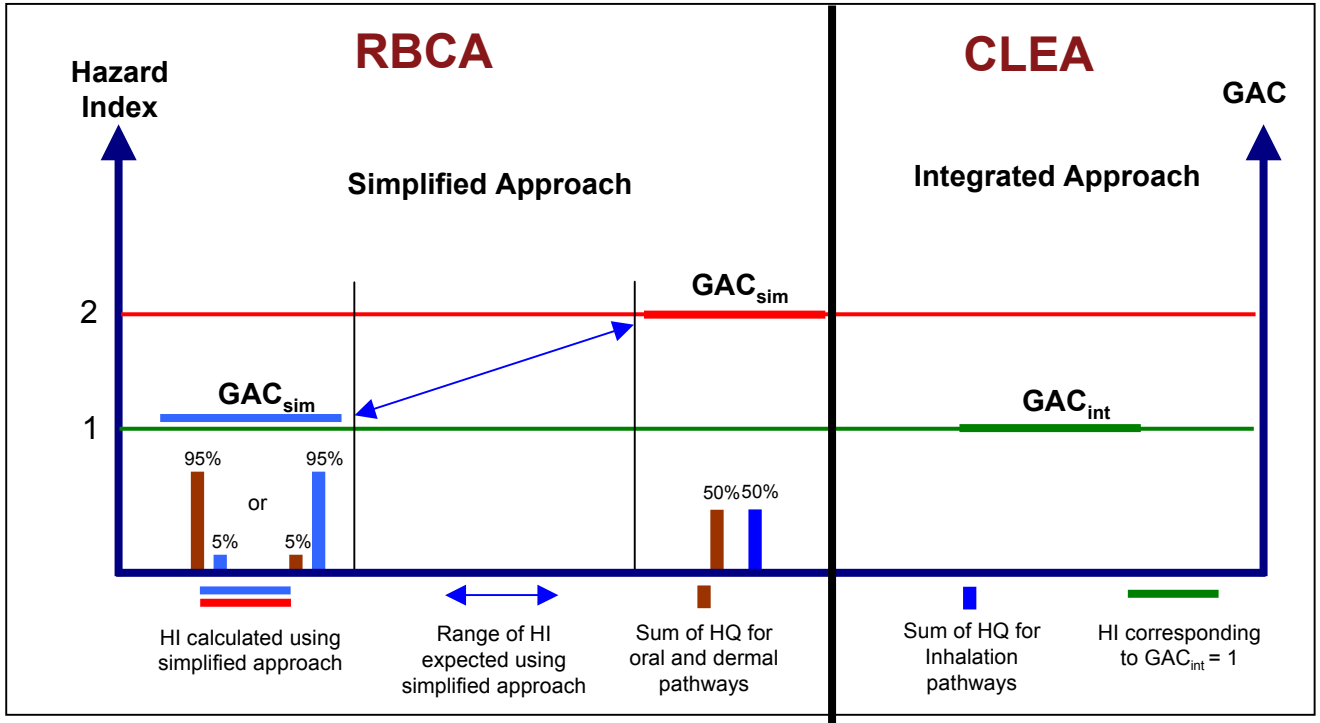


Model Limitations

- 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

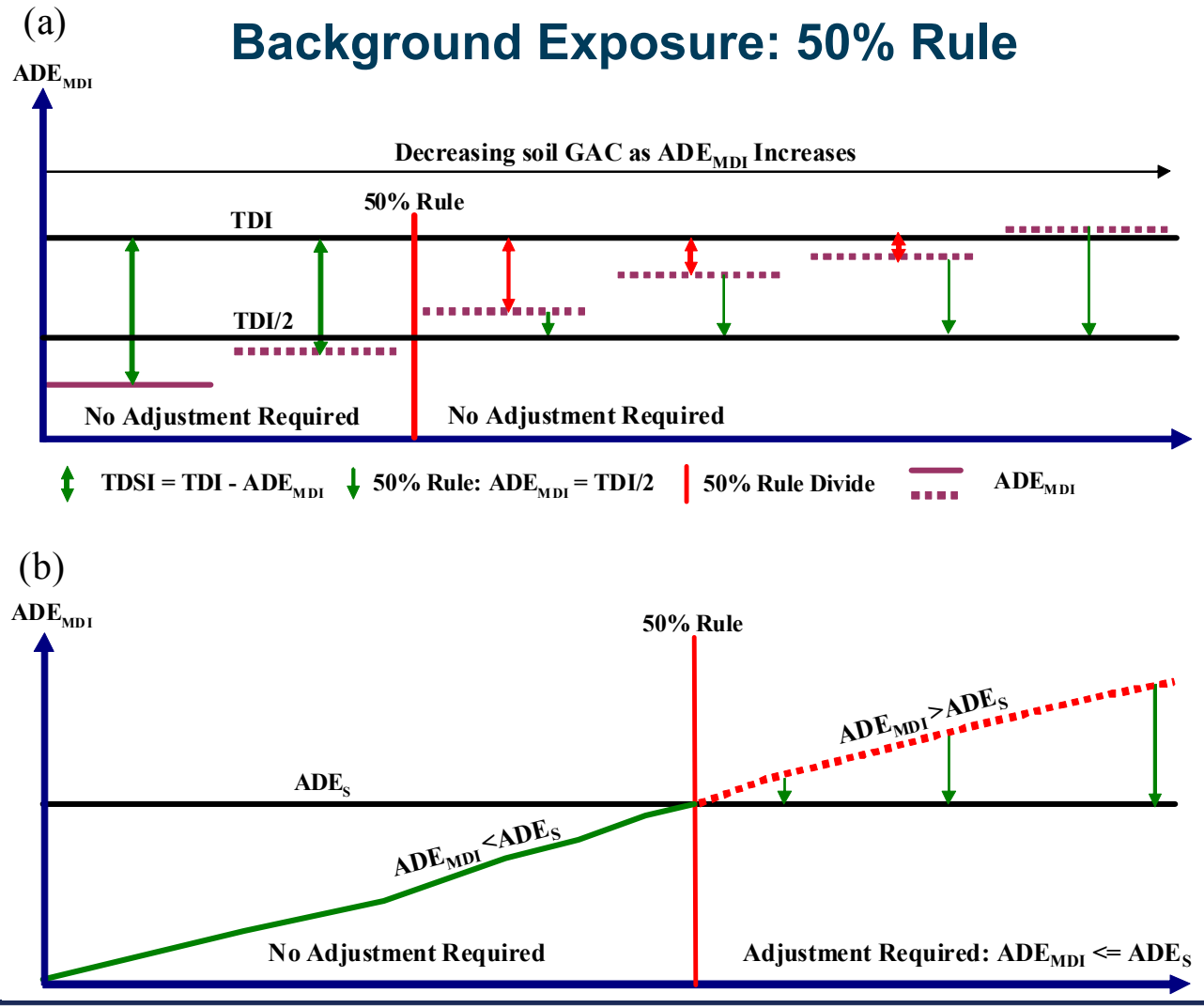


$$GAC = \min(GAC_{SS}, GAC_{ihn\_in}, GAC_{ihn\_out})$$

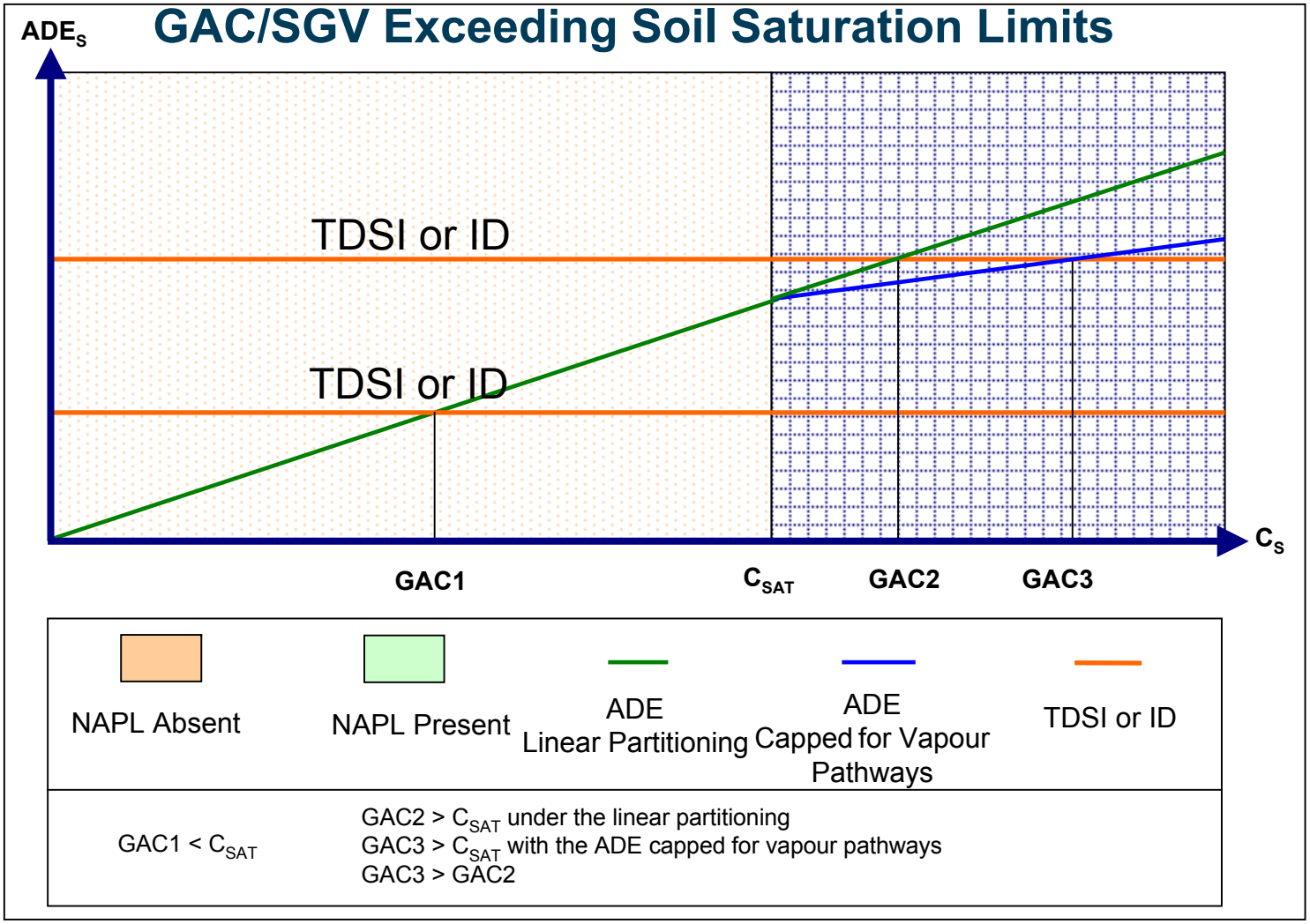
$$\frac{GAC_{\text{int}} \times \sum_{j=1}^{t}\sum_{o=1}^{m} R_o^j}{TDI^o - ADE_{MDI}^o} + \frac{GAC_{\text{int}} \times \sum_{j=1}^{t}\sum_{pv=1}^{n} R_{pv}^j}{TDI^i - ADE_{MDI}^i} = 1$$

Model Limitations

Background Exposure: 50% Rule



Model Limitations



Estimation of Human Exposure

Calculation of Average Daily Exposure (ADE)

$$\mathrm{ADE_s} = \sum_{j=1}^{t}\sum_{n=1}^{r}\frac{IR_j^n \times EF_j^n \times ED_j^n}{AT_j^n \times BW_j} = \mathrm{C_S} \times \sum_{j=1}^{t}\sum_{o=1}^{m} R_o^j + \mathrm{C_S} \times \sum_{j=1}^{t}\sum_{pv=1}^{n} R_{pv}^j$$

Calculation of Background Exposure

$$ADE_{MDI}^{o} = \mathrm{MDI^o} \times \sum_{j=1}^{t}\frac{EF \times ED \times CF_j^o}{AT \times BW_j} \qquad ADE_{MDI}^{i} = \mathrm{MDI}^i \times \sum_{j=1}^{t}\frac{EF \times ED \times CF_j^i}{AT \times BW_j}$$

Calculation of TOTAL Exposure

$$ADE_{S+MDI} = ADE_{MDI}^{o} + ADE_{MDI}^{i} + GAC_{\mathrm{int}} \times \left(\sum_{j=1}^{i}\sum_{o=1}^{m} R_o^j + \sum_{j=1}^{i}\sum_{pv=1}^{n} R_{pv}^j\right)$$

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^{o}_{MDI} >50% Oral TDI^{o}，Inhalation ADE^{i}_{MDI} <50% Inhalation TDI^{i}

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

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^{o}，Inhalation ADE^{i}_{MDI} >50% Inhalation TDI^{i}

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

CLEA solution: the Goal Seek Function

AIP: Solution of a Polynomial Equation

Estimation of Human Exposure

Equations to Calculate Generic Assessment Criteria for Soil

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

Scenario 3：Oral ADE^{o}_{MDI} >50% oral TDI^{o}，Inhalation ADE^{i}_{MDI} >50% Inhalation TDI^{i}

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

CLEA solution: the Goal Seek Function

AIP: Solution of a Polynomial Equation

Analytical Integration Procedures

TABLE 6. Summary of Integration Procedures in Presence of NAPL

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

$$GAC_{int} = \frac{e - f - hc}{b + \frac{a(e-f)}{(d-g)}} \qquad (13b)$$

Solution to Equation 10b (Limiting oral background exposure)

$$GAC_{int} = \frac{\frac{2ae - 2af + db - ahc}{ab} - \sqrt{\left(\frac{2ae - 2af + db - ahc}{ab}\right)^2 - 4 \times \frac{2de - 2df - dhc}{ab}}}{2} \qquad (14b)$$

Solution to Equation 11b (Limiting inhalation background exposure)

$$GAC_{int} = \frac{\frac{2db + ae - ahc - 2gb}{ab} - \sqrt{\left(\frac{2db + ae - ahc - 2gb}{ab}\right)^2 - 4 \times \frac{(d-g)(e-2hc)}{ab}}}{2} \qquad (15b)$$

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

$$GAC_{int} = \frac{\frac{2db + 2ae - 3ahc}{3ab} - \sqrt{\left(\frac{2db + 2ae - 3ahc}{3ab}\right)^2 - 4 \times \frac{(de - 2dhc)}{3ab}}}{2} \qquad (16b)$$

$$a = \sum_{j=1}^{t}\sum_{o=1}^{m} R_o^j \quad b = \sum_{j=1}^{t}\sum_{p=1}^{q} R_p^j \quad c = \sum_{j=1}^{t}\sum_{v=1}^{s} R_v^j \quad \mathbf{d = TDI^o} \quad \mathbf{e = TDI^i} \quad \mathbf{f = ADE^i_{MDI}} \quad \mathbf{g = ADE^o_{MDI}} \quad \mathbf{h = C_{int}}$$

HERA-Soil Model

TABLE 9. Comparison of the GAC_{int} Derived from the CLEA and HERA-Soil model

COC	Residential with Garden		Residential without Garden		Allotment		Commercial	
	CLEA	HERA	CLEA	HERA	CLEA	HERA	CLEA	HERA
Ethylbenzene	63.32	63.32	70.66	70.66	91.18	91.17	***7507.27***	120833
Xylene	32.55	32.55	33.49	33.49	173.42	173.37	***3833.31***	36381
Naphthalene	8.71	8.71	9.22	9.22	23.44	23.41	***1117.31***	49561
Carbon Tetrachloride	0.089	0.089	0.0899	0.0899	0.85	0.85	15.04	15.04
Cadmium	28.88	28.88	30.16	30.16	58.67	58.68	294.39	294.39
Nickel	110.45	110.49	113.16	113.17	246.65	246.66	989.13	989.17

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$_{dss}$