

Table_S5_supplement. Deterministic models, their availability and reactions that can be modelled

| Model | Geochemical Reactions | | | | | | | | Availability | | | Platform |
|------------------|-----------------------|-------|-----|---|----|------|-----------|---|----------------|------------|--------------|----------------------|
| | SOR | Ion-E | P/D | D | MO | BACT | NAPL-PART | OTHER | Free | Commercial | Cost (\$) | |
| 3DFATMIC | X | | X | X | X | X | | | X | | | DOS |
| BIOMOC3D | X | | | X | X | | | | X | | | DOS |
| BIOPLUME III | X | X | | X | X | X | | | X | | | Windows |
| BIOREDOX-MT3DMS | X | | | X | X | | | | X | | | DOS |
| BIOSLURP | X | | | X | | X | X | Sequential degradation | | X | | |
| Chain_2D | X | | | X | | | | Sequential 1 st -order degradation | X ^a | | | Fortran |
| CORT3D | X | | | X | | | | Oxidation of CEC by MNO_4^- | X | | | Windows |
| CTRAN and SEEP/W | X | | | X | | | | | | X | 6,450 | Windows |
| FEFLOW | X | | | X | | | | | | X | 0 – 2,200 | Windows |
| FEHM | X | X | X | X | X | | X | | X | | | Linux/MacOSX/Windows |
| Hydrus | X | X | X | X | X | X | | | | X | 630-6,000 | Windows |
| MT3D/MT3DMS | X | | | X | | | | 1 st -order degradation | X | | | DOS/ Windows |
| PFLOWTRAN | X | X | X | | X | | X | | X | | | Fortran, Linux |
| PHREEQC | X | X | X | X | X | X | X | | X | | | DOS/ Windows |
| PHT3D | X | X | X | X | X | X | X | | X | | | |
| RT3D | X | | | X | X | X | | | X | | | Windows |
| SEAM3D | X | | | X | X | X | | 1 st -order degradation | | X | 2,800-12,300 | Fortran |
| SUTRA | X | | | X | | | | | | X | | DOS/Unix |
| SWMS 2D/3D | X | | X | X | | | | 1 st -order degradation | X | | | Fortran |

| | | | | | | | | | | | | |
|-------------------------|---|---|---|---|---|---|---|---|---|---|--------------|--|
| TMVOC | X | | | X | | | X | | | X | 1,125-20,000 | |
| TOUGH2v2 and TOUGHREACT | X | X | X | X | | | | surface complexation is also coded | | | | |
| UTCHEM | X | X | X | X | X | X | X | Biodegradation is modelled as a 1 st order, instantaneous or Monod process | X | | | |

SOR - sorption, ION-E – ion exchange, P/D – precipitation, dissolution, D – degradation, MO – microbial oxidation, BACT – simulation of bacteria growth, /decay, NAPL – PART- NAPL partitioning, a – with GMS software