BIODEGRADATION MODELING BASED ON 14-COMPOUND GROUP KINETICS

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Petroleum biodegradation has traditionally been considered as a quasi-stepwise process that sequentially removes petroleum compounds of increasing stability or resistivity against microbial decomposition (Peters and Moldowan, 1993). Most microorganisms are substrate-specific and a number of complex metabolic pathways are used to derive energy from the petroleum constituents (Aitken *et al*., 2004; Annweiler *et al*., 2002; Heider *et al*., 1999; Zengler *et al*., 1999). Rather than proceeding strictly sequentially, it is likely that several metabolic pathways act in parallel but with different relative rates that are primarily controlled by the temperature regime. We have therefore implemented into the Biodexx tool a model that assumes simultaneous zero-order biodegradation reactions of different compound classes with different biodegradabilities and relative biodegradation rates.

Component	Number of C atoms	Biodegradability	Relative biodegradation rate
Methane	1	-	-
Ethane	2	+++	+
Propane	3	+++	+++
i-Butane	4	+++	++
n-Butane	4	+++	+++
i-Pentane	5	+++	++
n-Pentane	5	+++	++
n-Hexane	6	+++	++
PK_P10	7-14	++	+++
PK_P20	15-24	++	++
PK_P30	25-34	++	++
PK_P40	35-44	+	+
PK_P50	45-54	+	+
PK_P60+	55-80	+	+

Table 1 Components/compound classes with their characteristic number of carbon atoms (di Primio and Horsfield, 2006), relative biodegradabilities and relative biodegradation rates

The BioPetS concept aims at including biodegradation into oil quality prediction within the usual 3-D basin modeling process. We have therefore chosen to use one of the currently

most advanced kinetic petroleum generation concepts (di Primio and Horsfield, 2006) which is based on 14 compounds/compound classes and provides the capability of PVT-behavior prediction. Each compound or compound class is attributed a relative biodegradability (between 0 and 1) that determines which mass fraction can theoretically be removed by microbial attack. The second compound-specific parameter is the relative biodegradation rate: In a first step a field-wide maximum biodegradation rate has to be assessed for a given geologic setting as well as its variability with reservoir temperature. This biodegrading rate is a function of temperature and is assumed valid for the entire reservoir. The relative biodegradation rates of the individual compound groups are then normalized to and expressed as fractions of the field-wide biodegradation rate.

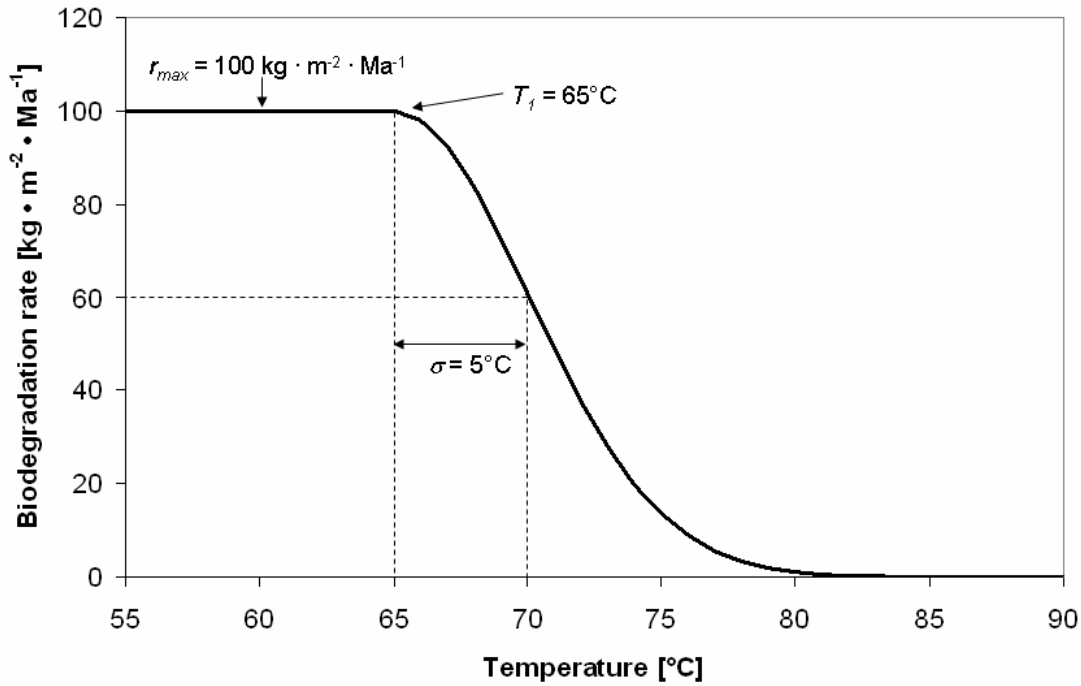

Fig. 1 Concept for biodegradation rates: constant biodegradation rate r_{max} with increasing temperature until a critical temperature T_1 is reached; above that temperature rates decrease in relation to σ ($r_{biodeg} = 0.61 \cdot r_{max}$ at $T = T_1 + \sigma$)

As the biodegradation process is not yet completely understood it is difficult to predict biodegradation in completely unexplored areas. We have therefore chosen a post-processor approach where results from basin modeling (masses and compositions of inflowing oil, geometric information, temperatures etc.) are imported into the Biodexx module. It is thus possible to quickly check different biodegradation scenarios by varying maximum biodegradation rates as these might range within several orders of magnitude (Larter *et al*., 2003).

The Biodexx concepts and the workflow will be presented with selected examples.

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