MODA

Physics-based Model: Electronic – Statistical charge transport – Fermi Golden Rule hopping model (RoMM 1.6.2)

1	**ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED**	
1.1	**ASPECT OF THE USER CASE TO BE SIMULATED**	Transport of electrons between coarse grained representations of molecules.
1.2	**MATERIAL**	*P3HT:PCBM, PCDTBT:PCBM, etc*
1.3	**GEOMETRY**	*Up to 100x100x100* nm^3 *domains containing the bulk heterojunction*
1.4	**TIME LAPSE**	*up to ms*
1.5	**MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS**	
1.6	**PUBLICATION ON THIS DATA**	

2	**GENERIC PHYSICS OF THE MODEL EQUATION**		
2.0	**MODEL TYPE AND NAME**	Statistical charge transport model	
2.1	**MODEL ENTITY**	Electrons	
2.2	**MODEL PHYSICS/ CHEMISTRY EQUATION PE**	**Equation**	Semi-classical Marcus charge transport theory in the high temperature limit.
		Physical quantities	Charge, current density and field profiles.
2.3	**MATERIALS RELATIONS**	**Relation**	Charge transfer (hopping) rates based on Fermi's Golden Rule: $\omega_{ij} = \frac{J_{ij}}{\hbar}\sqrt{\frac{\pi}{\lambda_{ij} k_B T}}\exp\left(-\frac{(\Delta E_{ij} - \lambda_{ij})^2}{4\lambda_{ij} k_B T}\right)$

		Physical quantities/ descriptors for each MR	Reorganization energies (λ_{ij}), site energy differences (ΔE_{ij}), electronic coupling elements (J_{ij}), charge transfer rates (ω_{ij}).
2.4	**SIMULATED INPUT**	From CGMD: Coarse grain molecular geometry. From DFT: Reorganization energies, site energy differences, electronic couplings.	

3	**SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS**		
3.1	**NUMERICAL SOLVER**	Kinetic Monte Carlo	
3.2	**SOFTWARE TOOL**	In-house KMC solver.	
3.3	**TIME STEP**		
3.4	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	Site occupation probability p_i obeys the steady state rate equation $\frac{\partial p_i}{\partial t} = -\sum_j\left[\omega_{ij}p_i(1-p_j) - \omega_{ji}p_j(1-p_i)\right] = 0$. Waiting time for an event step between sites *i* and *j* is $\tau_{ij} = -\frac{\ln(r)}{\omega_{ij}}$, where *r* is a random number (0,1).
3.5	**COMPUTATIONAL BOUNDARY CONDITIONS**	Electrostatic bias across simulation cell	
3.6	**ADDITIONAL SOLVER PARAMETERS**		

4	**POST PROCESSING**
4.1	**THE PROCESSED OUTPUT**	Current density, carrier mobility Output (carrier mobility) will be used in larger finite volume simulations of continuum electrics (drift-diffusion).
4.2	**METHODOLOGIES**	Current density is obtained from carrier flux, charge mobility from drift velocity of carriers in an external field.
4.3	**MARGIN OF ERROR**	