

Class 16

Particle Reactions

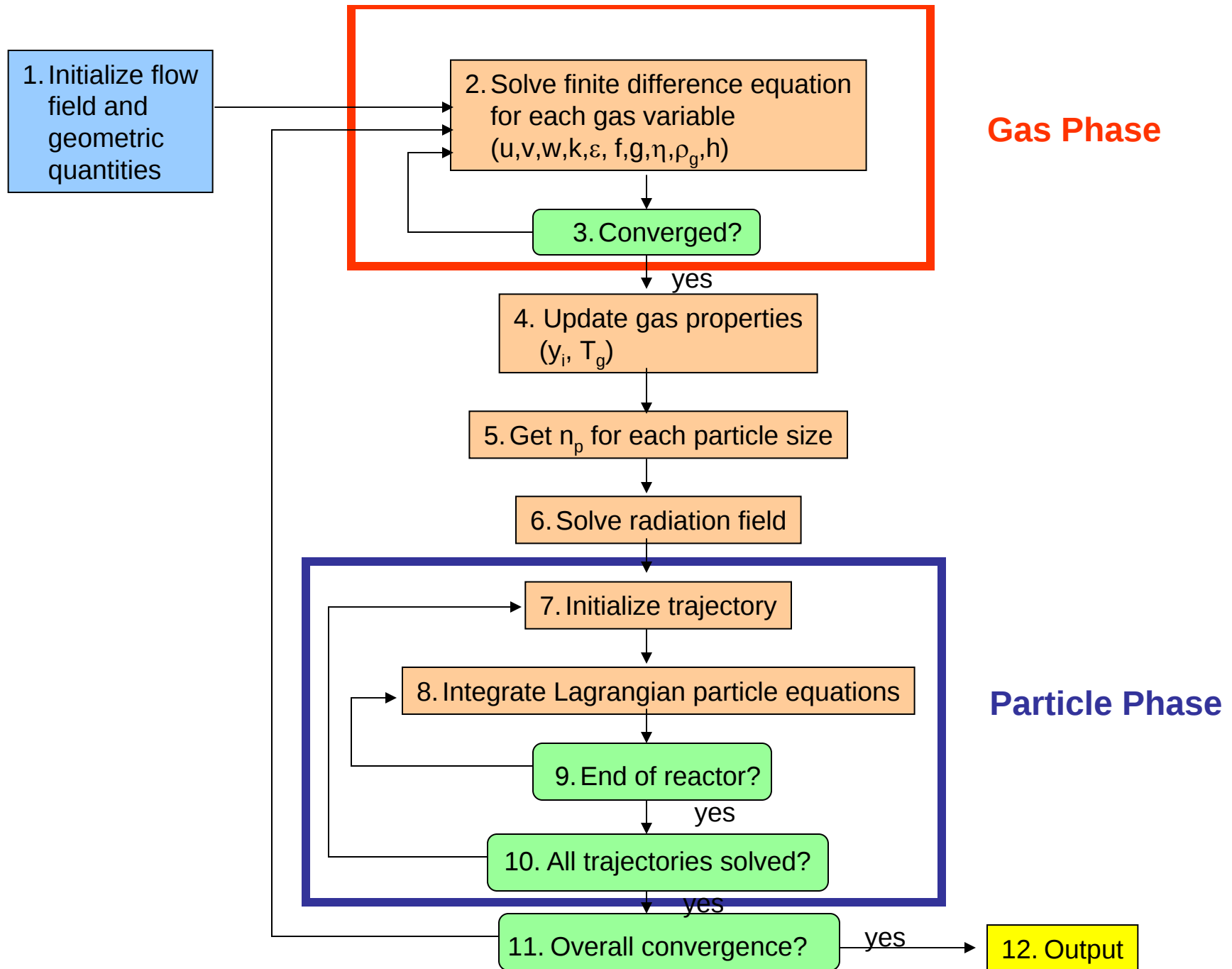
Table 2.6: Convective and Conductive Heat Transfer for Particle Model

Type	Equation
Particle enthalpy	$h_j = \frac{\alpha_{wj}h_{wj} + \alpha_{cj}h_{cj} + \alpha_{hj}h_{hj} + \alpha_{aj}h_a}{\alpha_j} \quad (2.125)$
Particle-gas heat transfer	$Q_i = Nu_{jg} \pi \left(\frac{B_j}{\exp B_j - 1} \right) k_g (T_j - T_g) d_j \quad (2.126)$
Nusselt No.	$Nu_{jg} = 2.0 + 0.65 Re_{jg}^{0.5} Pr_g^{0.333} \quad (2.127)$
Transpiration parameter	$B_j = \frac{r_j C_{pg}}{2\pi d_j k_g} \quad (2.128)$
Reynolds No.	$Re_{jg} = \frac{d_j \left \vec{v}_g - \vec{v}_j \right \rho_g}{\mu_g} \quad (2.129)$
Prandtl No.	$Pr_g = \frac{C_{pg} \mu_g}{k_g} \quad (2.130)$
Liquid enthalpy	$h_{wj} = h_{fwj}^0 + \int_{298}^{T_j} C_{pwj} dT_j \quad (2.131)$
Raw coal enthalpy	$h_{cj} = h_{fcj}^0 + \int_{298}^{T_j} C_{pcj} dT_j \quad (2.132)$
Char enthalpy	$h_{hj} = h_{fhj}^0 + \int_{298}^{T_j} C_{phj} dT_j \quad (2.133)$
Ash enthalpy	$h_{aj} = h_{faj}^0 + \int_{298}^{T_j} C_{paj} dT_j \quad (2.134)$
Volatiles enthalpy	$h_{vjm} = \frac{h_{cj} - h_{hj}(1 - Y_{jm})}{Y_{jm}} \quad (2.135)$
Total particle product gas enthalpy	$h_{jg} = \frac{1}{r} \left[\sum_m r_{vjm} h_{vjm} + h_{hj} \sum_l r_{hjl} + r_{wj} h_{wj} \right. \\ \left. + \zeta \left(\sum_m r_{vjm} \Delta h_{jm}^r + \sum_l r_{hjl} \Delta h_{jl}^r + r_{wj} \Delta h_w^v \right) \right] \quad (2.136)$
Particle heat of formation	$h_{fj}^o = \frac{\alpha_{wj}h_{fwj}^o + \alpha_{hj}h_{fhj}^o + \alpha_{cj}h_{fcj}^o + \alpha_{aj}h_{fa}^o}{\alpha_j} \quad (2.137)$

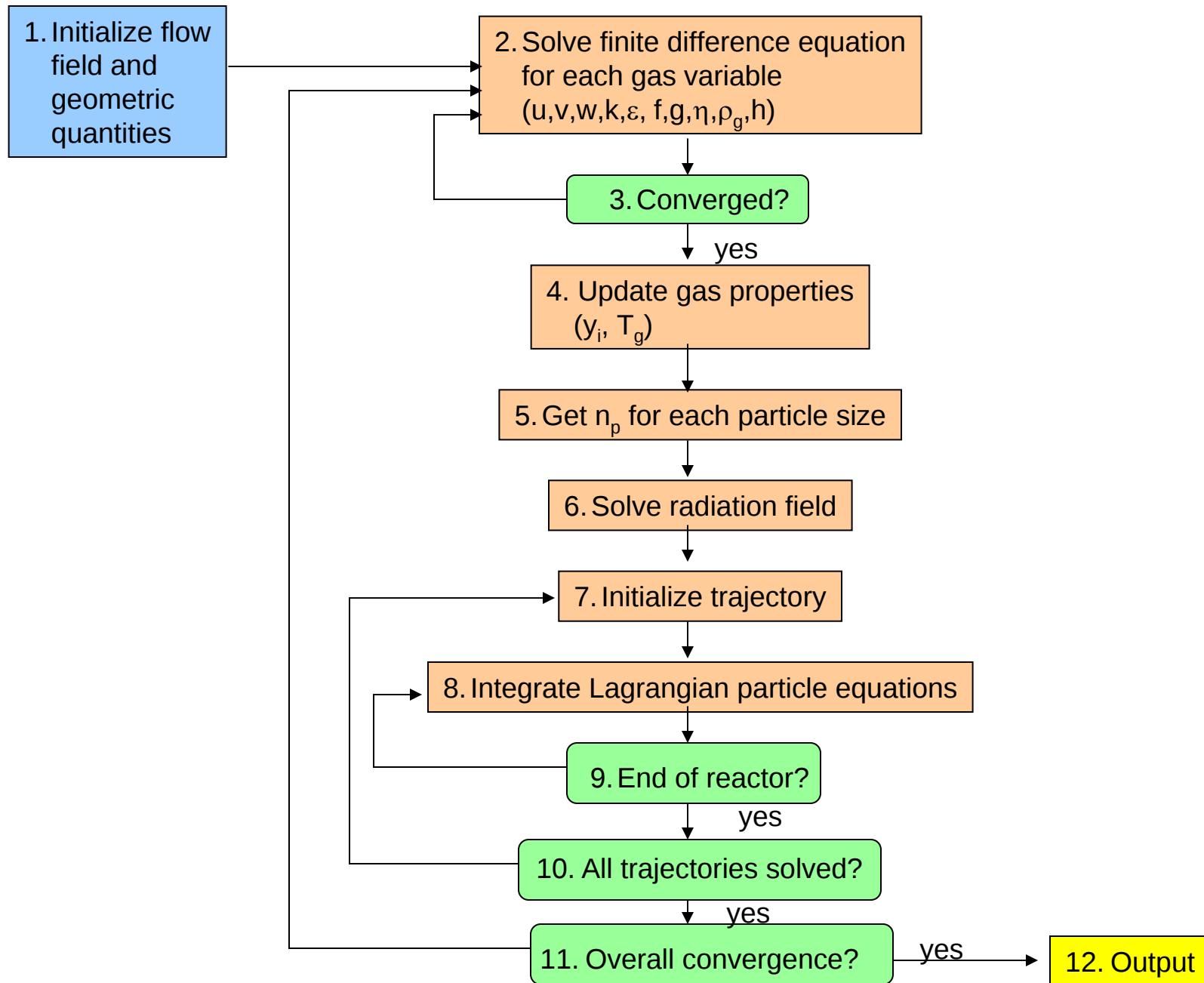
from corrected 1993 PCGC-3 User's Manual

Table 2.7: Particle Reactions for Particle Model

Type	Equation
Liquid vaporization rate (non-boiling)	$r_{wj} = \frac{S_f A_j k_{jw} \rho_g (X_{wjs} - X_{wb}) + X_{wjs} \sum_m S_f r_{vjm}}{1 - X_{wjs}} \quad (2.139)$
Liquid vaporization rate (boiling)	$r_{wj} = \frac{-Q_j + Q_{rj} + r_{cj} (h_{jg} - h_{cj}) \zeta + r_{hj} \zeta (h_{jg} - h_{hj})}{\zeta (h_{jg} - h_{wj})} \quad (2.140)$
Particle reaction rate to gas phase	$r_j = \sum_l r_{hjl} + \sum_m r_{vjm} + r_{wj} \quad (2.141)$
Net char reaction rate	$r_{hj} = \sum_m r_{hjm} - \sum_l r_{hjl} \quad (2.142)$
Oxidizer-char reaction rate	$r_{hjl} = \frac{A_j^2 M_{hj} M_g \phi_l k_{cji} k_{jl} \zeta_j C_{olg} C_g}{M_g A_j C_g (\zeta_j k_{jl} - k_{cjl}) + r_j} \quad (2.143)$
Kinetic char reaction rate coefficient	$k_{jl} = A_{jl} T_j^n \exp\left(\frac{-E_{jl}}{RT_j}\right) \quad (2.144)$
Transpiration parameter for mass transfer	$B_{jl} = \frac{r_j}{2\pi D_{im} \rho_g d_j} \quad (2.145)$
Mass transfer coefficient	$k_{cji} = \frac{Sh_{jg} D_{im} B_{ji}}{d_j (\exp B_{ji} - 1)} \quad (2.146)$
Total coal reaction rate	$r_{cj} + \sum_m -r_{cjm} = -\sum_m (r_{hjm} + r_{vjm}) \quad (2.417)$
Volatile production rate	$r_{vjm} = k_{mj} Y_{mj} \alpha_{cj} \quad (2.418)$
Char production rate	$r_{hjm} = \frac{r_{vjm} (1 - Y_{mj})}{Y_{mj}} \quad (2.419)$
Coal kinetic rate coefficient	$k_{mj} = A_{mj} \exp\left(\frac{-E_{mj}}{RT_j}\right) \quad (2.150)$



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