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Reaction Fronts in a Porous Medium. Approximation Techniques versus Numerical Solution

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The flame sheet approximation (FS) and a novel polynomial approximation technique (PA) are compared in terms of their capability to describe reaction fronts of highly exothermic reactions in a porous medium. A one-phase model and a two-phase model of a system with adiabatic walls and a radiant output (to approximate the case of a porous radiant burner) are included in the analysis. By matching the reaction zone solution found by either the FS or PA method with the solutions of the non reacting zones, the temperature, conversion, and position of the reaction zone were determined. Numerical solutions for catalytic and non catalytic oxidation reactions were used to compare the predictions of both approaches. It was found that although both techniques yielded good approximations to the solutions, the PA technique proved to be more accurate, producing results with 3.5% of the numerical results. Both methods can find useful application in the analysis of this class of problems.

$$T_{\mathrm{f}} = T_{\mathrm{f0}} + \frac{1}{\gamma} T_{\mathrm{f1}} + \dots \tag{1}$$

$$\gamma = \frac{E}{R T_{\mathrm{f0}}} \tag{2}$$

$$v = x\gamma \tag{3}$$

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$$\Theta\left(x_i, y_i, \frac{\mathrm{d}y_i}{\mathrm{d}x}, \ldots, \frac{\mathrm{d}^{n-1}y_i}{\mathrm{d}x^{n-1}}, \frac{\mathrm{d}^n y_i}{\mathrm{d}x^n}\right) = 0, \quad (k + 1 \text{ equations}) \qquad (4)$$

$$S\left(\Delta x_j, y_j, \frac{\mathrm{d}y_j}{\mathrm{d}x}, \ldots, \frac{\mathrm{d}^n y_j}{\mathrm{d}x^n}\right) = 0, \quad (\mathrm{k} - 1 \text{ equations}) \qquad (7)$$

$$x_{i+1} = x_i + \Delta x_i, \quad (k \text{ equations}) \qquad (8)$$

$$L_\mathrm{t} = x_k - x_0, \quad (1 \text{ equation}) \qquad (9)$$

$$g_0\left(x_0, y_0, \frac{\mathrm{d}y_0}{\mathrm{d}x}, \ldots, \frac{\mathrm{d}^{n-1}y_0}{\mathrm{d}x^{n-1}}\right) = 0, \quad n_1 \ (n_1 \text{ equations}, n_1 < n) \qquad (5)$$

$$g_k\left(x_k, y_k, \frac{\mathrm{d}y_k}{\mathrm{d}x}, \ldots, \frac{\mathrm{d}^{n-1}y_k}{\mathrm{d}x^{n-1}}\right) = 0, \quad (n - n_1 \text{ equations}) \qquad (6)$$

$$f_i(x, y, C_1, C_2, \ldots, C_n) = 0 \qquad (10)$$

$$(r_1 + 1) + (r_3 + 1) + (s - 1)(r_2 + 1) = sn + m + 1 \qquad (11)$$

$$m = n + s \qquad (12)$$

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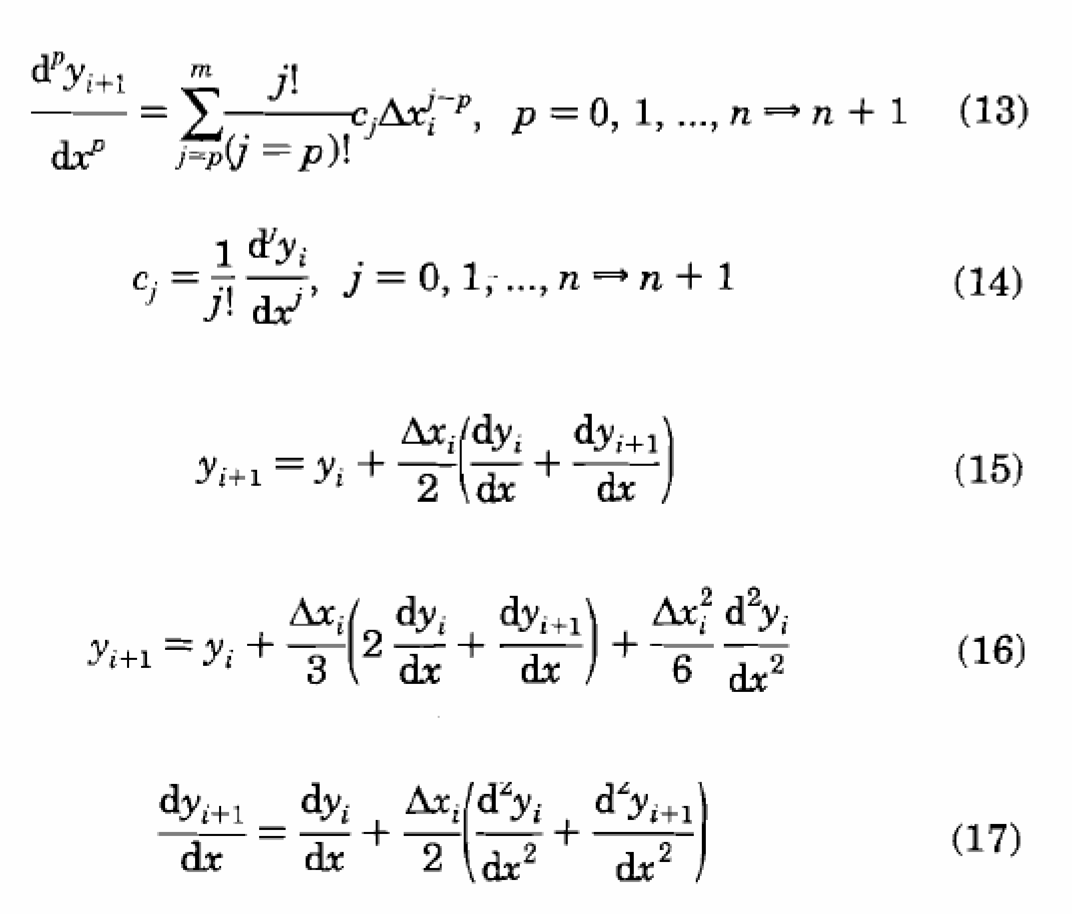

$$\frac{d^p y_{i+1}}{dx^p} = \sum_{j=p}^{m} \frac{j!}{(j = p)!} c_j \Delta x_i^{j-p}, \quad p = 0, 1, ..., n \Rightarrow n + 1 \qquad (13)$$

$$c_j = \frac{1}{j!}\frac{d^j y_i}{dx^j}, \quad j = 0, 1, ..., n \Rightarrow n + 1 \qquad (14)$$

$$y_{i+1} = y_i + \frac{\Delta x_i}{2}\left(\frac{dy_i}{dx} + \frac{dy_{i+1}}{dx}\right) \qquad (15)$$

$$y_{i+1} = y_i + \frac{\Delta x_i}{3}\left(2\frac{dy_i}{dx} + \frac{dy_{i+1}}{dx}\right) + \frac{\Delta x_i^2}{6}\frac{d^2 y_i}{dx^2} \qquad (16)$$

$$\frac{dy_{i+1}}{dx} = \frac{dy_i}{dx} + \frac{\Delta x_i}{2}\left(\frac{d^2 y_i}{dx^2} + \frac{d^2 y_{i+1}}{dx^2}\right) \qquad (17)$$

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$$y_{i+q} = y_i + q\frac{\Delta x_{j+i}}{6(1+r)}\left[(3+2r)\frac{dy_{i+q}}{dx} + (1+r)(3+r)\frac{dy_i}{dx} - r^2\frac{dy_{i-q}}{dx}\right] \quad (18)$$

where

$$r = \left(\frac{\Delta x_{i+1}}{\Delta x_i}\right)^q, \quad q = \pm 1, \quad j = \frac{1}{2}(q-1) \qquad (19)$$

The two additional equations for the fourth order polynomial PA(2,2) are

$$\frac{dy_{i+q}}{dx} = \frac{dy_i}{dx} + q\frac{\Delta x_{j+i}}{6(1+r)}\left[(3+2r)\frac{d^2y_{i+q}}{dx^2} + (1+r)(3+r)\frac{d^2y_i}{dx^2} - r^2\frac{d^2y_{i-q}}{dx^2}\right] \quad (20)$$

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$$y_{i+q} = y_i + q\frac{\Delta x_{j+i}}{2}\left(\frac{\mathrm{d}y_i}{\mathrm{d}x} + \frac{\mathrm{d}y_{i+q}}{\mathrm{d}x}\right) + \frac{\Delta x_{j+i}^2}{12}\left(\frac{\mathrm{d}^2 y_i}{\mathrm{d}x^2} - \frac{\mathrm{d}^2 y_{i+q}}{\mathrm{d}x^2}\right) \qquad (21)$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[(k_\mathrm{e} + bT^3)\frac{\mathrm{d}T}{\mathrm{d}x}\right] - GC_p\frac{\mathrm{d}T}{\mathrm{d}x} + (-\Delta H)\mathbf{R} = 0 \qquad (22)$$

$$\frac{\mathrm{d}w}{\mathrm{d}x} = -\frac{\mathbf{R}}{G} \qquad (23)$$

$$\mathbf{R} = k_*\frac{w}{T}\mathrm{e}^{-E/RT} \qquad (24)$$

$$k_* = \frac{\epsilon k_0 \Pi}{R} \qquad (25)$$

$$(k_\mathrm{e} + bT^3)\frac{\mathrm{d}T}{\mathrm{d}x} = GC_p(T - T_\mathrm{in}) \qquad (26)$$

$$w = w_\mathrm{in} \qquad (27)$$

$$(k_\mathrm{e} + bT^3)\frac{\mathrm{d}T}{\mathrm{d}x} = h_\mathrm{r}(T_\mathrm{w}{}^4 - T^4) \qquad (28)$$

$$-cx = b\left[z^2(T_j - T) - \frac{z}{2}(T_j^2 - T^2) + \frac{1}{3}(T_j^3 - T^3)\right] + (k_e - bz^3)\ln\left(\frac{z + T_j}{z + T}\right) \quad (29)$$

where

$$c = GC_p \quad (30)$$

$$T_j = T_1, \quad z = -T_{in} \quad (31)$$

$$\frac{dT_1}{dx} = \frac{c}{k_e + bT_1^3}(T_1 - T_{in}) \quad (32)$$

For zone II

$$T_j = T_k, \quad z = \frac{k_e + bT_k^3}{c}\frac{dT_k}{dx} - T_k \quad (33)$$

$$\frac{dT_k}{dx} = \frac{c}{k_e + bT_k^3}\left[T_k - T_{k+1} - \frac{h_r}{c}(T_{k+1}^4 - T_w^4)\right] \quad (34)$$

$$T_{f1} = \gamma(T_1 - T_{f0}) \quad \text{and} \quad \frac{dT_{f1}}{d\upsilon} = \frac{dT_1}{dx} \quad (35)$$

when $\upsilon \to +\infty$, ($T = T_k$, $w = w_{out}$)

$$T_{f1} = (T_k - T_{f0}) \quad \text{and} \quad \frac{dT_{f1}}{d\upsilon} = \frac{dT_k}{dx} \quad (36)$$

$$\frac{dT_1}{dx} - \frac{dT_k}{dx} = \beta_{in} - \beta_{out} \quad (37)$$

$$\frac{d^2T_{f1}}{d\upsilon^2} = -a\left(\frac{dT_{f1}}{d\upsilon} - \frac{dT_k}{dx} + \beta_{out}\right)e^{T_{f1}/T_m} \quad (38)$$

$$\beta_{in,out} = \frac{(-\Delta H)}{k_e + bT_m^3}Gw_{in,out} \quad (39)$$

$$a = \frac{\epsilon k_0 \Pi e^{-E/RT_m}}{GE} \quad (40)$$

$$\frac{\mathrm{d}T_{\mathrm{fl}}}{\mathrm{d}v} - \frac{\mathrm{d}T_1}{\mathrm{d}x} + \left(\frac{\mathrm{d}T_k}{\mathrm{d}x} - \beta_{\mathrm{out}}\right) \ln\left(\frac{\frac{\mathrm{d}T_{\mathrm{fl}}}{\mathrm{d}v} - \frac{\mathrm{d}T_k}{\mathrm{d}x} + \beta_{\mathrm{out}}}{\beta_{\mathrm{in}}}\right) = -aT_{\mathrm{m}}(\mathrm{e}^{T_{\mathrm{fl}}/T_{\mathrm{m}}} - \mathrm{e}^{\gamma(T_1 - T_{\mathrm{m}})/T_{\mathrm{m}}}) \quad (41)$$

By taking the limit $v \rightarrow +\infty$ in eq 41, we get

$$\frac{\mathrm{d}T_k}{\mathrm{d}x} - \frac{\mathrm{d}T_1}{\mathrm{d}x} + \left(\frac{\mathrm{d}T_1}{\mathrm{d}x} - \beta_{\mathrm{in}}\right) \ln\left(\frac{w_{\mathrm{out}}}{w_{\mathrm{in}}}\right) = -aT_{\mathrm{m}} \times (\mathrm{e}^{\gamma(T_k - T_{\mathrm{m}})/T_{\mathrm{m}}} - \mathrm{e}^{\gamma(T_1 - T_{\mathrm{m}})/T_{\mathrm{m}}}) \quad (42)$$

At $v = 0$, $T = T_{\mathrm{m}}$ and $\mathrm{d}T_{\mathrm{fl}}/\mathrm{d}v = 0$; eq 41 yields

$$-\frac{\mathrm{d}T_1}{\mathrm{d}x} + \left(\frac{\mathrm{d}T_1}{\mathrm{d}x} - \beta_{\mathrm{in}}\right) \ln\left(1 - \frac{\mathrm{d}T_1/\mathrm{d}x}{\beta_{\mathrm{in}}}\right) = -aT_{\mathrm{m}}(1 - \mathrm{e}^{\gamma(T_1 - T_{\mathrm{m}})/T_{\mathrm{m}}}) \quad (43)$$

$$G^2 = \frac{\epsilon k_0 \Pi}{E}[T_{\mathrm{m}}(k_{\mathrm{e}} + bT_{\mathrm{m}}{}^3)\mathrm{e}^{-E/RT_{\mathrm{m}}}(1 - \mathrm{e}^{-E(T_{\mathrm{m}} - T_0)/RT_{\mathrm{m}}{}^2})]/\left[C_p(T_{\mathrm{m}} - T_{\mathrm{in}}) + [w_{\mathrm{in}}(-\Delta H) - C_p(T_{\mathrm{m}} - T_{\mathrm{in}})] \times \ln\left[1 - \frac{C_p(T_{\mathrm{m}} - T_{\mathrm{in}})}{w_{\mathrm{in}}(-\Delta H)}\right]\right] \quad (44)$$

$$\frac{\mathrm{d}^2 T_i}{\mathrm{d}x^2} = \frac{1}{k_{\mathrm{e}i}}\left[-3b\left(T_i \frac{\mathrm{d}T_i}{\mathrm{d}x}\right)^2 + c\frac{\mathrm{d}T_i}{\mathrm{d}x} - (-\Delta H)\frac{k_* w_i}{T_i}\mathrm{e}^{-E/RT_i}\right] \quad (45)$$

$$w_i \doteq w_{\mathrm{in}} - \frac{1}{G(-\Delta H)}\left[c(T_i - T_{\mathrm{in}}) - k_{\mathrm{e}i}\frac{\mathrm{d}T_i}{\mathrm{d}x}\right] \quad (46)$$

$$\frac{\mathrm{d}^2 T_i}{\mathrm{d}x^2} = \Theta\left(T_i, \frac{\mathrm{d}T_i}{\mathrm{d}x}\right), \quad i = 1, 2, ..., k \quad (47)$$

$$\frac{\mathrm{d}w_i}{\mathrm{d}x} = v_1 \frac{\mathrm{d}w_2}{\mathrm{d}x} \quad \text{and} \quad \frac{\mathrm{d}w_k}{\mathrm{d}x} = v_k \frac{\mathrm{d}w_2}{\mathrm{d}x} \quad (48)$$

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$$k_e \frac{d^2 T_s}{dx^2} = h_s(T_s - T_g) - \Psi(-\Delta H)\mathbf{R}_s \qquad (49)$$

$$-GC_p \frac{dT_g}{dx} + h_s(T_s - T_g) + (1 - \Psi)(-\Delta H)\mathbf{R}_g = 0 \qquad (50)$$

$$\frac{dw}{dx} = -\Psi \frac{\mathbf{R}_s}{G} - (1 - \Psi)\frac{\mathbf{R}_g}{G} \qquad (51)$$

$$\mathbf{R}_s = k_* \frac{w}{T_s} e^{-E/RT_s} \quad \text{and} \quad \mathbf{R}_g = k_* \frac{w}{T_g} e^{-E/RT_g} \qquad (52)$$

$$k_e \frac{dT_s}{dx} = h_0(T_s - T_{in}) \qquad (53)$$

$$T_g = T_{in} + \frac{h_0}{GC_p}(T_s - T_{in}) \qquad (54)$$

$$w = w_{in} \qquad (55)$$

$$k_e \frac{dT_s}{dx} = h_r(T_w^4 - T^4) + h_c(T_g - T_s) \qquad (56)$$

$$T_g = C + Ae^{Mx} + Be^{Nx} \qquad (57)$$

$$T_s = C + Af_m e^{Mx} + Bf_n e^{Nx} \qquad (58)$$

$$M, N = \frac{h_s}{2c}\left[-1 \pm \left(1 + \frac{4c^2}{k_e h_s}\right)^{1/2}\right], \quad M > N \qquad (59)$$

$$f_m = 1 + \frac{cM}{h_s}, \quad f_n = 1 + \frac{cN}{h_s} \qquad (60)$$

$$C = T_{in} \qquad (61)$$

$$A = \frac{T_{g1} - T_{in}}{e^{-ML_1} - e^{-NL_1}}(\Gamma - e^{-NL_1}) \qquad (62)$$

$$B = \frac{T_{g1} - T_{in}}{e^{-ML_1} - e^{-NL_1}}(-\Gamma + e^{-ML_1}) \qquad (63)$$

$$\Gamma = \frac{(N-M)\dfrac{h_0}{h_s}}{\left(1-\dfrac{h_0}{c}-\dfrac{h_0}{h_s}M\right)e^{NL_1}-\left(1-\dfrac{h_0}{c}-\dfrac{h_0}{h_s}N\right)e^{ML_1}} \tag{64}$$

$$T_{s1} = T_{in} + f_m A + f_n B \tag{65}$$

$$\frac{dT_{g1}}{dx} = \frac{h_s}{c}(T_{s1} - T_{g1}) \tag{66}$$

$$\frac{dT_{s1}}{dx} = \frac{c}{k_e}(T_{g1} - T_{in}) \tag{67}$$

$$T_g = T_{in} + (T_{g1} - T_{in})e^{Mx} \tag{68}$$

$$T_s = T_{in} + (T_{g1} - T_{in})f_m e^{Mx} \tag{69}$$

$$T_{s1} = T_{in} + f_m(T_{g1} - T_{in}) \tag{70}$$

$$C = T_{gk} - \frac{k_e}{c}\frac{dT_{sk}}{dx} \tag{71}$$

$$A = \frac{c\dfrac{dT_{gk}}{dx} - k_e N\dfrac{dT_{sk}}{dx}}{c(M-N)}; \quad B = \frac{-c\dfrac{dT_{gk}}{dx} + k_e M\dfrac{dT_{sk}}{dx}}{c(M-N)} \tag{72}$$

$$\frac{dT_{gk}}{dx} = \frac{h_s}{c}(T_{sk} - T_{gk}) \tag{73}$$

$$k_e\frac{dT_{s(k+1)}}{dx} = h_c(T_{g(k+1)} - T_{s(k+1)}) - h_r({T_{s(k+1)}}^4 - {T_w}^4) \tag{74}$$

$$T_{g(k+1)} = C + Ae^{ML_2} + Be^{NL_2} \tag{75}$$

$$T_{s(k+1)} = C + Af_m e^{ML_2} + Bf_n e^{NL_2} \tag{76}$$

$$\frac{dT_{s(k+1)}}{dx} = AMf_m e^{ML_2} + BNf_n e^{NL_2} \tag{77}$$

$$T_g = T_{gf0} + \frac{1}{\gamma}T_{gf1} + \dots \tag{78}$$

$$T_s = T_{sf0} + \frac{1}{\gamma}T_{sf1} + \dots \tag{79}$$

$$w = w_{\mathrm{f0}} + \frac{1}{\gamma} w_{\mathrm{f1}} + \dots \tag{80}$$

$$\frac{\mathrm{d}^2 T_{\mathrm{sf0}}}{\mathrm{d}v^2} = 0, \quad \rightarrow \frac{\mathrm{d}T_{\mathrm{sf0}}}{\mathrm{d}v} = \text{constant} \tag{81}$$

$$k_{\mathrm{e}} \frac{\mathrm{d}^2 T_{\mathrm{sf1}}}{\mathrm{d}v^2} = -\Psi(-\Delta H) \frac{k_*' w_{\mathrm{f0}}}{T_{\mathrm{sf0}}} \mathrm{e}^{-E/RT_{\mathrm{s}}} \tag{82}$$

$$c \frac{\mathrm{d}T_{\mathrm{gf0}}}{\mathrm{d}v} = (1 - \Psi)(-\Delta H) \frac{k_*' w_{\mathrm{f0}}}{T_{\mathrm{gf0}}} \mathrm{e}^{-E/RT_{\mathrm{s}}} \tag{83}$$

$$\frac{\mathrm{d}w_{\mathrm{f0}}}{\mathrm{d}v} = -\frac{k_*' w_{\mathrm{f0}}}{G} \left[\frac{\Psi}{T_{\mathrm{sf0}}} \mathrm{e}^{-E/RT_{\mathrm{s}}} + \frac{1 - \Psi}{T_{\mathrm{gf0}}} \mathrm{e}^{-E/RT_{\mathrm{g}}} \right] \tag{84}$$

$$k_*' = k_*/\gamma \tag{85}$$

$$\mathrm{d}T_{\mathrm{sf1}}/\mathrm{d}v = \text{constant} \tag{86}$$

$$w_{\mathrm{f0}} = w_{\mathrm{in}} - \frac{C_p}{(-\Delta H)} (T_{\mathrm{gf0}} - T_{\mathrm{g1}}) \tag{87}$$

$$\frac{\mathrm{d}T_{\mathrm{g}}}{\mathrm{d}x} = \frac{k_*}{G T_{\mathrm{g}}} \left[\frac{(-\Delta H) w_{\mathrm{in}}}{C_p} + T_{\mathrm{g1}} - T_{\mathrm{g}} \right] \mathrm{e}^{-E/RT_{\mathrm{g}}} \tag{88}$$

$$h_{\mathrm{s}}(T_{\mathrm{s1}} - T_{\mathrm{g1}}) = \frac{k_*(-\Delta H) w_{\mathrm{in}}}{T_{\mathrm{g1}}} \mathrm{e}^{-E/RT_{\mathrm{g1}}} \tag{89}$$

$$T_{\mathrm{gm}} = T_{\mathrm{g1}} + (-\Delta H) w_{\mathrm{in}}/C_p \tag{90}$$

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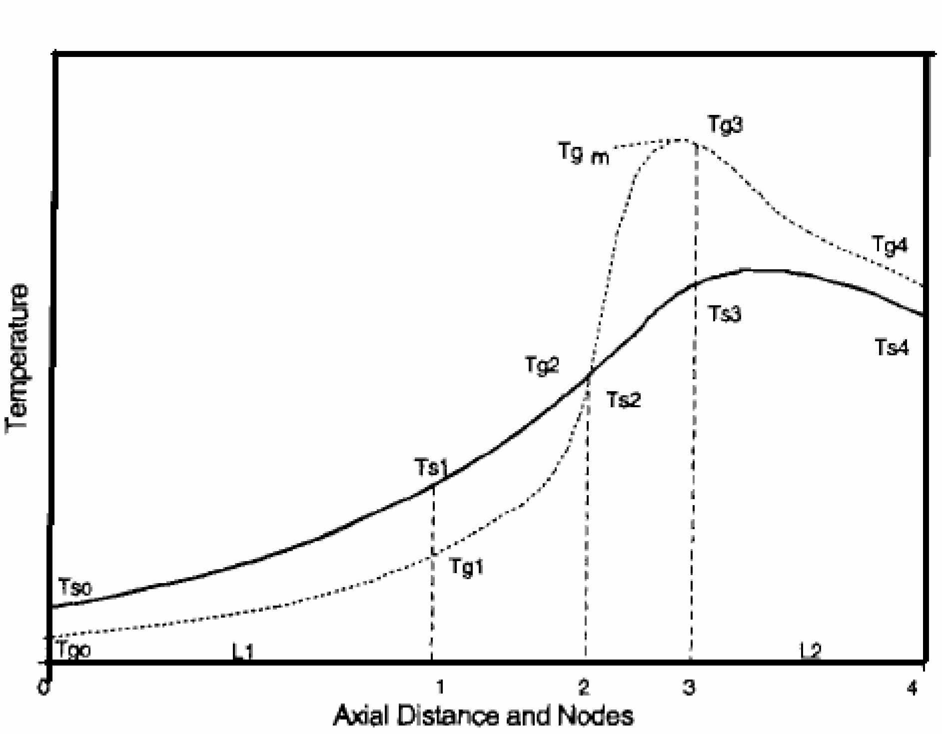

Figure 1. Integration steps for the two-phase model (burner).

$$\frac{\mathrm{d}T_{s1}}{\mathrm{d}x} - \frac{\mathrm{d}T_{sk}}{\mathrm{d}x} = \beta_{\mathrm{in}} - \beta_{\mathrm{out}} \tag{91}$$

$$\frac{\mathrm{d}T_{sk}}{\mathrm{d}x} - \frac{\mathrm{d}T_{s1}}{\mathrm{d}x} + \left(\frac{\mathrm{d}T_{s1}}{\mathrm{d}x} - \beta_{\mathrm{in}}\right)\ln\left(\frac{w_{\mathrm{out}}}{w_{\mathrm{in}}}\right) = -\alpha T_{\mathrm{m}}\left(\mathrm{e}^{\gamma(T_{s(k+1)}-T_{\mathrm{m}})/T_{\mathrm{m}}} - \mathrm{e}^{\gamma(T_{s0}-T_{\mathrm{m}})/T_{\mathrm{m}}}\right) \tag{92}$$

$$G^2 = \frac{\epsilon k_0 \Pi}{E}[T_{\mathrm{m}} k_{\mathrm{e}} \mathrm{e}^{-E/RT_{\mathrm{m}}}(1 - \mathrm{e}^{-E(T_{\mathrm{m}}-T_{s0})/RT_{\mathrm{m}}^2})]\Big/\left[C_p(T_{g1} - T_{\mathrm{in}}) + [w_{\mathrm{in}}(-\Delta H) - C_p(T_{g1} - T_{\mathrm{in}})]\ln\left[1 - \frac{C_p(T_{g1} - T_{\mathrm{m}})}{w_{\mathrm{in}}(-\Delta H)}\right]\right] \tag{93}$$

$$\frac{\mathrm{d}^2T_{si}}{\mathrm{d}x^2} = \frac{h_s}{k_{\mathrm{e}}}(T_{si} - T_{gi}) - \Psi\frac{(-\Delta H)k_* w_i}{k_{\mathrm{e}} T_{si}}\mathrm{e}^{-E/RT_{si}} \tag{94}$$

$$\frac{\mathrm{d}T_{gi}}{\mathrm{d}x} = \frac{1}{c}\left[h_s(T_{si} - T_{gi}) + (1 - \Psi)\frac{(-\Delta H)k_* w_i}{k_{\mathrm{e}} T_{gi}}\mathrm{e}^{-E/RT_{gi}}\right] \tag{95}$$

$$w_i = w_{\mathrm{in}} + \frac{1}{G(-\Delta H)}\left[c(T_{\mathrm{in}} - T_{gi}) + k_{\mathrm{e}}\frac{\mathrm{d}T_{si}}{\mathrm{d}x}\right] \tag{96}$$

$$\frac{\mathrm{d}^2T_{si}}{\mathrm{d}x^2} = \Theta_s\left(T_{si}, \frac{\mathrm{d}T_{si}}{\mathrm{d}x}, T_{gi}\right) \tag{97}$$

$$\frac{\mathrm{d}T_{gi}}{\mathrm{d}x} = \Theta_g\left(T_{si}, \frac{\mathrm{d}T_{si}}{\mathrm{d}x}, T_{gi}\right) \tag{98}$$

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$$|h_s(T_{si} - T_{gi})| = \zeta|(-\Delta H)G\frac{dw_i}{dx}|, \quad \zeta > 0 \qquad (99)$$

$$T_{gk} = T_{in} + \frac{(-\Delta H)w_{in}}{C_p} + \frac{k_e}{c}\frac{dT_{sk}}{dx} \qquad (100)$$

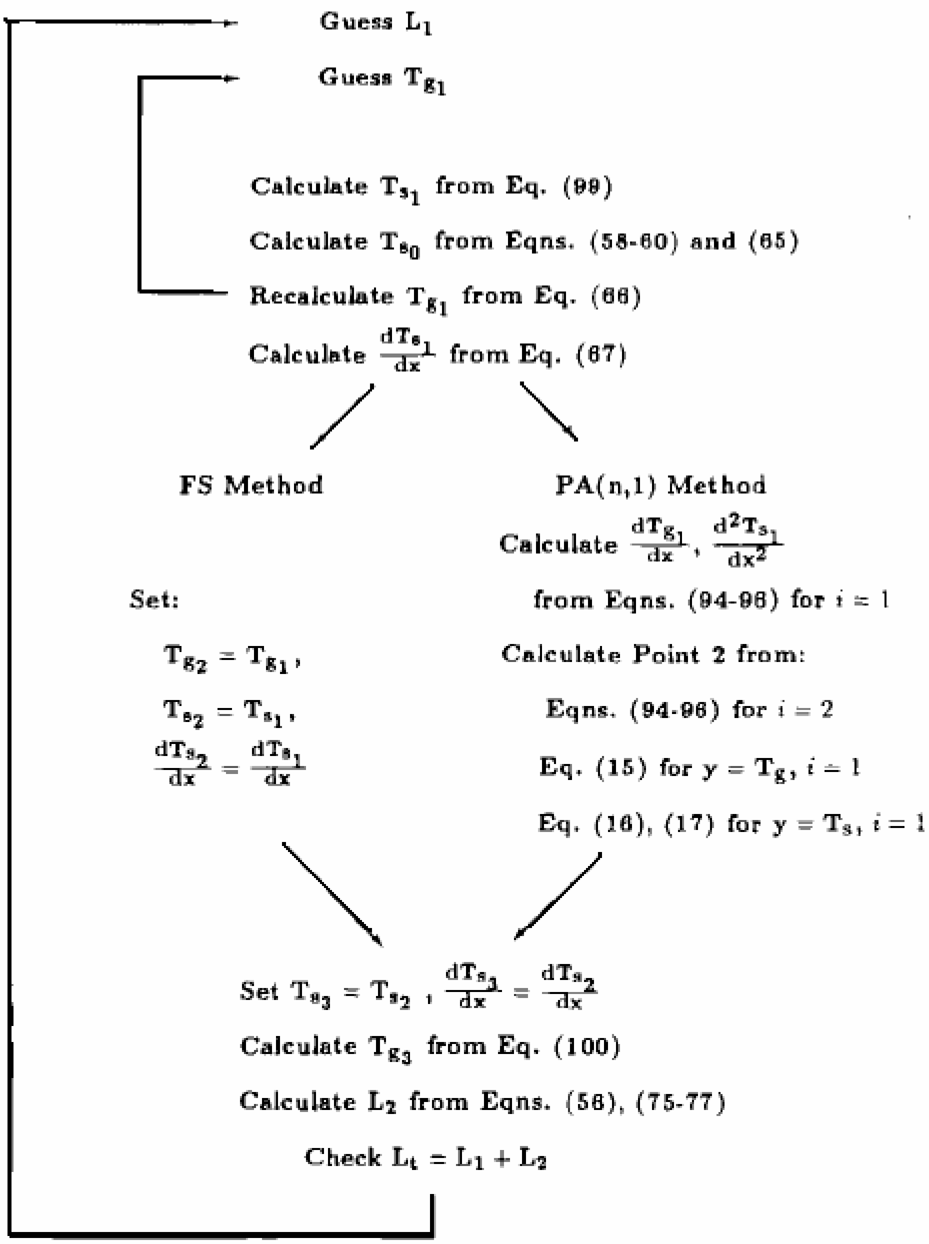

Figure 2. Calculation scheme to solve the PRB model.

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Table 1. Parameter Values

		CO oxidation		CH$_4$ combustion	
parameter	units	1-phase	2-phase	1-phase	2-phase
b	W/(m·K^4)	1.0×10^{-9}		8.7×10^{-10}	
C_p	J/(mol·K)	30	30	40	45
E/R	K	11524	11524	15000	15000
G	mol/(s·m^2)	5.0	5.0	10.0	10.0
h_0	W/(m^2·K)		10		10
h_c	W/(m^2·K)		10		10
h_r	W/(m^2·K^4)			5.7×10^{-8}	5.7×10^{-8}
h_s	W/(m^3·K)		20000		200000
k_0	s^{-1}	1.12×10^{10}	1.12×10^{10}	1.8×10^{8}	1.8×10^{8}
k_e	W/(m·K)	4.0	4.0	1.5	2.5
L_t	m	0.10	0.10	0.04	0.04
T_{in}	K	427	427	300	300
w_{in}		0.03	0.03	0.08	0.08
$-\Delta H$	J/mol	2.8×10^{5}	2.8×10^{5}	8.0×10^{5}	8.0×10^{5}
ϵ		0.4	0.4	0.9	0.9
Π	atm	1.0	1.0	1.0	1.0

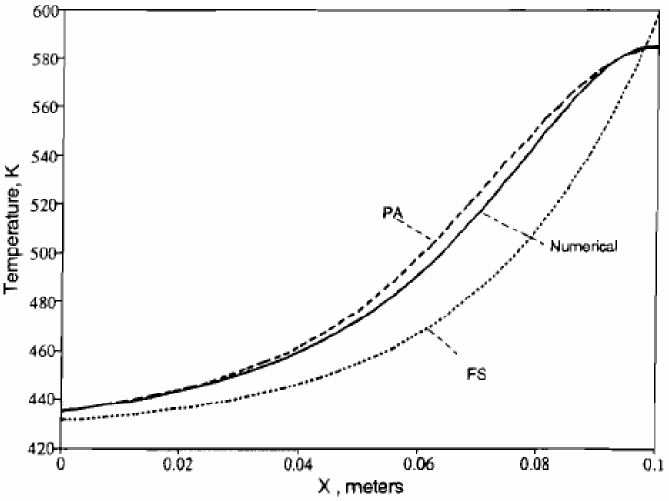

Figure 3. Comparison of temperature profiles. CO oxidation one-phase model.

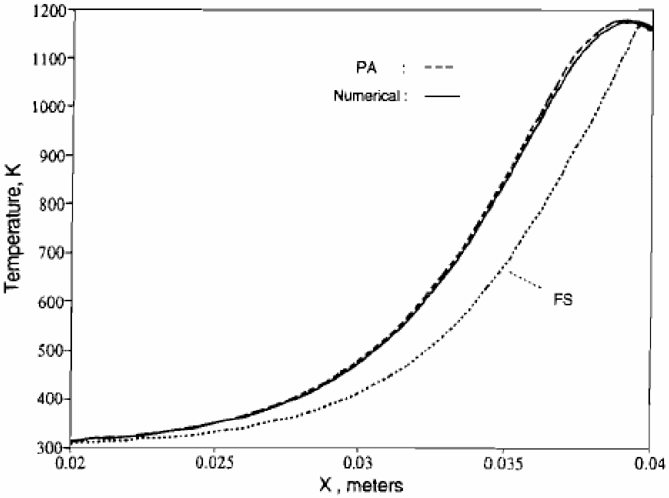

Figure 4. Comparison of temperature profiles. CH$_4$ oxidation, one-phase model.

Table 2. Comparison of Results for CO Oxidation[a]

				FS		PA	
model	G	variable at outlet	numer results	values	% error	values	% error
1-phase	2	temp	503.5	513.4	12.9%	500.9	−3.4%
		conv	27.3%	30.9%	13.0%	26.4%	−3.3%
	5	temp	585.3	598.1	8.1%	584.7	−0.4%
		conv	56.5%	61.1%	8.1%	56.3%	−0.4%
	10	temp	662.7	675.7	5.5%	664.0	0.6%
		conv	84.2%	88.8%	5.5%	84.6%	0.6%
2-phase	2	temp solid	503.0	510.7	10.1%	503.1	0.1%
		temp gas	502.8	507.2	5.8%	502.8	0.0%
		conv	27.1%	28.9%	6.6%	27.1%	−0.0%
	5	temp solid	573.1	578.1	3.4%	574.6	1.0%
		temp gas	566.1	549.9	−11.6%	565.6	−0.4%
		conv	49.8%	44.6%	−10.6%	49.7%	−0.3%
	10	temp solid	613.1	611.6	−0.8%	615.8	1.5%
		temp gas	570.7	537.4	−23.2%	573.6	2.0%
		conv	51.8%	40.3%	−22.2%	52.8%	2.0%

[a] The relative deviation for temperature values is found from % error = $100(T_{calc} - T_{numer})/(T_{numer} - T_{in})$.

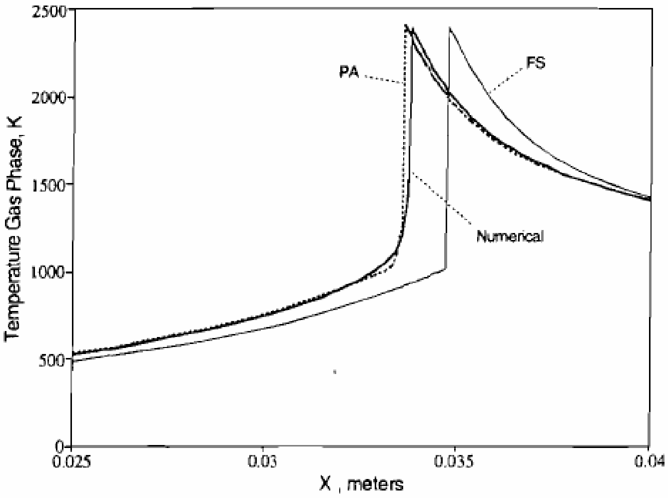

Figure 5. Comparison of temperature profiles. CH_4 oxidation, two-phase model.

Table 3. Comparison of Results for CH_4 Combustion[a]

				FS		PA	
model	param	item	numer results	values	% error	values	% error
1-phase	$G = 2$	T_{max}	920.81	921.2	0.1%	922.3	0.2%
		L_1	0.0336	0.0394	17.3%	0.0334	−0.6%
		conv	60.2%	60.8%	1.0%	60.2%	0.1%
	$G = 10$	T_{max}	1172.1	1168.7	−0.4%	1177.9	0.7%
		L_1	0.0391	0.0395	1.0%	0.0391	0.0%
		conv	69.3%	68.9%	−0.5%	69.9%	0.9%
	$G = 20$	T_{max}	1324.8	1317.3	−0.7%	1336.6	1.2%
		L_1	0.0396	0.0397	0.3%	0.0395	−0.3%
		conv	76.5%	75.7%	−1.0%	77.6%	1.5%
2-phase and $h_s = 200\,000$	$G = 5$	$T_{g(k+1)}$	1456.0	1502.6	4.0%	1464.4	0.7%
		$T_{s(k+1)}$	1031.8	991.1	−5.6%	1024.8	−1.0%
		L_1	0.0388	0.0389	0.2%	0.0388	−0.2%
	$G = 10$	$T_{g(k+1)}$	1401.5	1414.9	1.2%	1400.0	−0.1%
		$T_{s(k+1)}$	1265.4	1252.7	−1.3%	1266.6	0.1%
		L_1	0.0339	0.0384	2.6%	0.0336	−0.7%
	$G = 12$	$T_{g(k+1)}$	1423.7	1424.0	0.0%	1423.6	−0.0%
		$T_{s(k+1)}$	1300.2	1299.3	−0.1%	1300.1	−0.0%
		L_1	0.0233	0.0278	19.3%	0.0233	0.0%
2-phase and $G = 10$	$h_s = 120\,000$	$T_{g(k+1)}$	1406.6	1407.3	0.1%	1406.6	0.0%
		$T_{s(k+1)}$	1260.6	1260.0	−0.1%	1260.6	0.0%
		L_1	0.0173	0.0230	33.1%	0.0181	4.5%
	$h_s = 400\,000$	$T_{g(k+1)}$	1450.4	1485.2	3.0%	1447.5	−0.3%
		$T_{s(k+1)}$	1217.2	1179.1	−4.2%	1220.2	0.3%
		L_1	0.0382	0.0384	0.6%	0.0381	−0.3%

[a] The relative deviation for temperature values is found from % error = $100(T_{calc} - T_{numer})/(T_{numer} - T_{in})$.

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$$\mathrm{RE} = \frac{\text{heat released by radiation at output}}{\text{heat released by complete combustion}} \times 100 \qquad (101)$$

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Nomenclature

A = constant, eqs 62 and 72a
a = constant, eq 40
B = constant, eqs 63 and 72b
$b = 4\phi\sigma_B d_p$, W/(m·K^4)
C = constant, eqs 61 and 71
$c = GC_p$, W/(K·m^2)
C_p = specific heat of gas phase, J/(mol·K)
d_p = particle size in bed, m
E = activation energy, J/mol
f_m/f_n = parameters, eq 60
G = molar flux, mol/(s·m^2)
h = heat transfer coefficient, W/(m^2·K)
h_r = radiation heat transfer coefficient, W/(m^2·K^4)
h_s = interphase heat transfer coefficient, W/(m^3·K)
$(-\Delta H)$ = heat of reaction, J/mol
k_e = thermal conductivity, W/(m·K)
k_0 = frequency factor, s^{-1}
k_*, k_*' = parameters, eqs 25 and 85
L_t = length of reactor, m
L_1, L_2 = distances from flame to either bed end, m
M, N = roots of characteristic equation, eq 59
m, n = order of polynomial and differential equatic
R = universal gas constant, J/(mol·K)
$\mathbf{R}$ = reaction rate, mol/(s·m^3)
RE = radiant efficiency, eq 101
T = temperature, K
v = expanded axial distance, m
w = reactant molar fraction
x = axial distance, m
Δx = step size, m
z = parameter, eqs 31b and 34

Greek Symbols

β = parameter, eq 39
$\gamma = E/RT_{g0}$
Γ = parameter, eq 64
ϵ = bed porosity
ϕ = radiation transfer factor
Π = absolute inlet pressure, atm
σ_B = Stefan–Boltzmann constant, W/(m^2·K^4)
Ψ = parameter to distinguish between cases
ζ = constant, eq 99

Subscripts

0 = Beginning of bed
1 = Beginning of reaction zone
c = convective
f = inner expansion
g = gas phase
in = inlet
k = end of reaction zone
$k + 1$ = downstream end of bed
m = maximum value
out = outlet
s = Solid phase