Class 6

Simple Coal Devolatilization Models

Outline

- 1-step
- 2-step
- DAEM
- Compare capabilities
- Blowing Factor
- Bateman video
- Discuss effects of blowing

1-Step Model

$$\frac{dV}{dt} = k(V_{\infty} - V)$$

- V = % of coal that becomes volatiles
- V_{∞} = "Ultimate" yield (yield at infinite time)
- k = Arrhenius rate constant {A exp(-E/RT)}

2-Competing Step Model

$$\text{Coal} \rightarrow (1-Y_1)\ \text{Char}_1 + Y_1 V_1$$

$$\text{Coal} \rightarrow (1-Y_2)\ \text{Char}_2 + Y_2 V_2$$

$$\frac{dCoal}{dt} = -(k_1 + k_2)Coal$$

$$\frac{dV}{dt} = \frac{dV_1}{dt} + \frac{dV_2}{dt} = (Y_1 k_1 + Y_2 k_2)Coal$$

- Advantage: Heating rate effect on both rate and yield

Ubhayaker Coefficients

(buried in a figure)

cal process may correspond to less ... $_n = X_{O,n}$

tion, with consequent rupturing of unsaturated = 0.

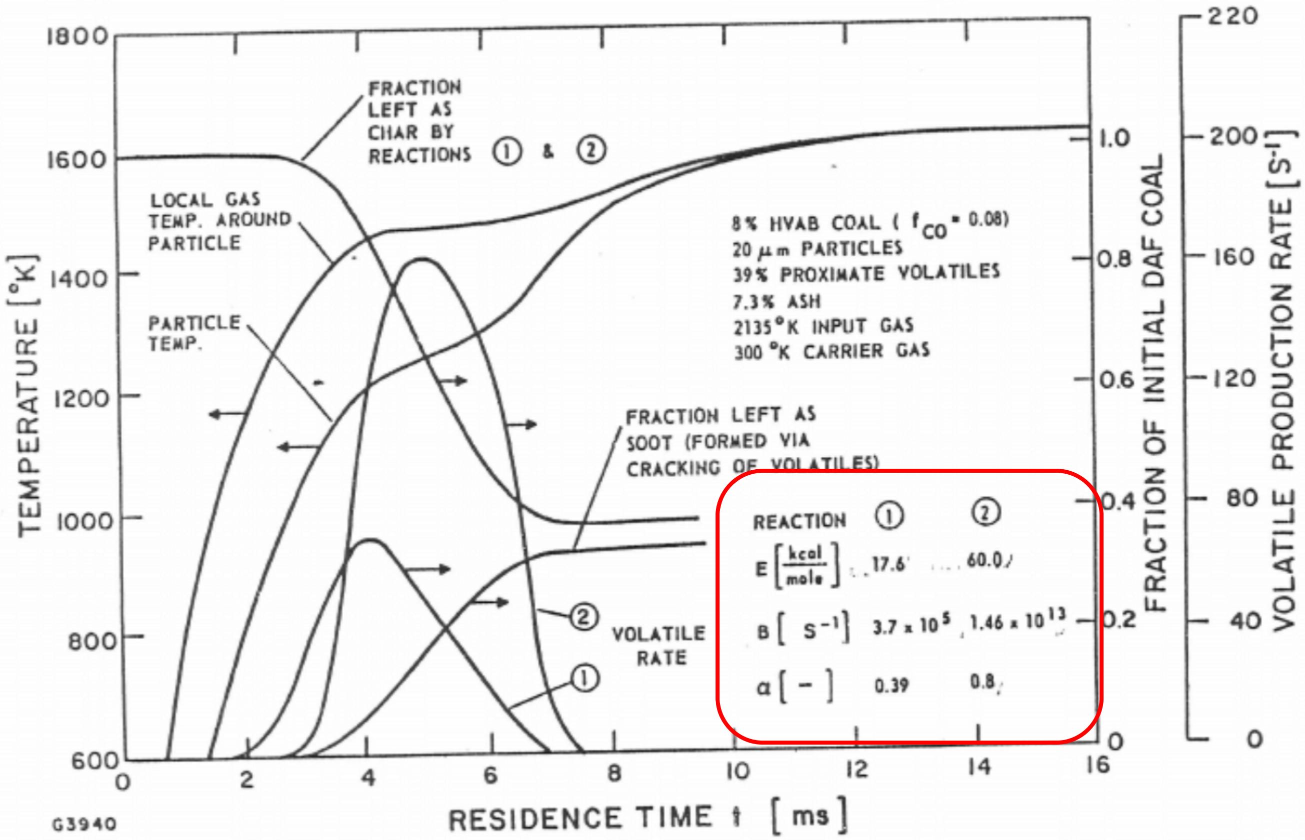


FIG. 2. Numerical solution to the analytical model evaluated for a monodisperse pulverized coal sample. The kinetic parameters were obtained by curve fitting the data of Kimber and Gray[3] and Badzioch and Hawksley.[4]

From Ubhayakar, et al., 16th Symp. (Int.) on Comb. p. 430 (1976).

Distributed Activation Energy Model (DAEM)

$$\frac{V_\infty - V}{V_\infty} = \int_0^\infty e^{-\int_0^t k dt} F(E) dE$$

$$F(E) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(E-E_0)^2}{2\sigma^2}}$$

- Assumption: Volatiles can be released from bins of different activation energy in parallel
- Advantage: Heating rate effect on rate
- Derivative form available

How do you solve the DAEM?

Gaussian quadrature!

$$\int_{-1}^{1} f(x)dx = \sum w_i\, f(x_i)$$

- Break up activation energies into 5 to 10 bins
- Quadrature theory tells what the weighting functions are
- Like 5 to 10 parallel reactions weighted appropriately

Series Distributed Activation Energy

- Concept of an effective E
- E_{eff} changes according to the distribution function:

$$E_{eff} = f(V, V_{\infty}, \sigma)$$

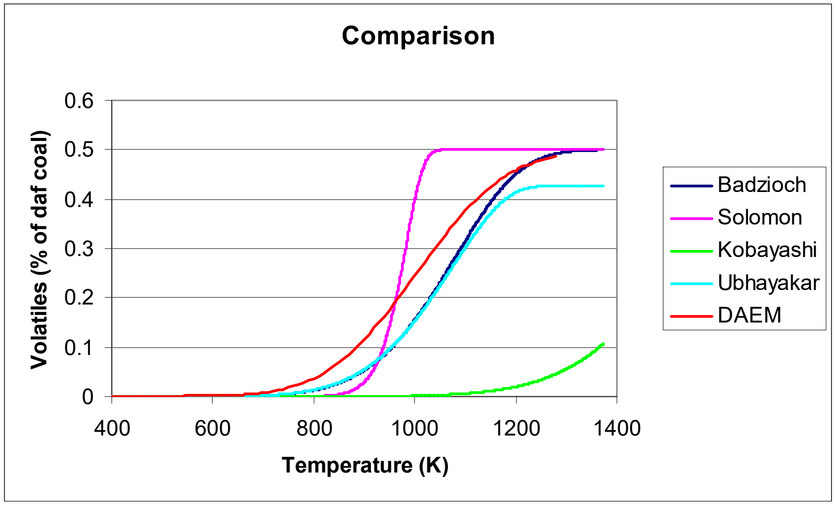
- E_{eff} changes according to a Gaussian distribution based on extent of conversion

$$\frac{dV}{dt} = k_{eff}(V_{\infty} - V)$$

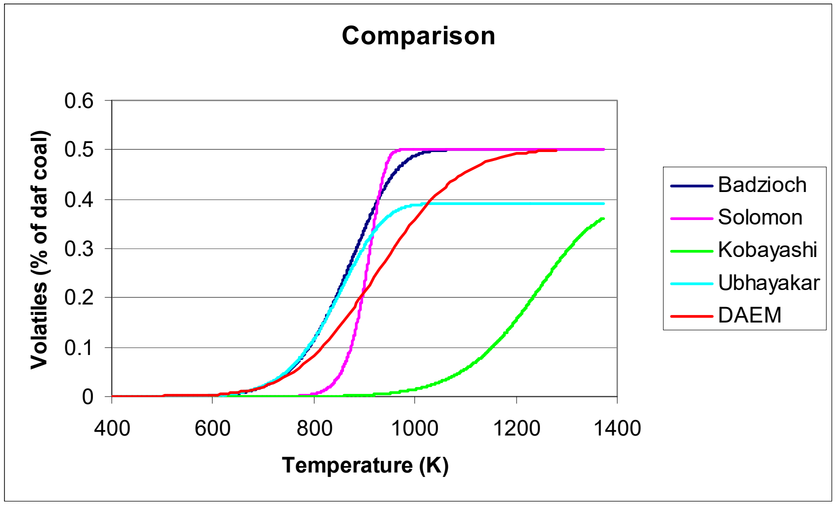
$$k_{eff} = Ae^{-\frac{E_{eff}}{RT}}$$

- MUCH faster with great results

Comparison of Coal Devolatilization Models

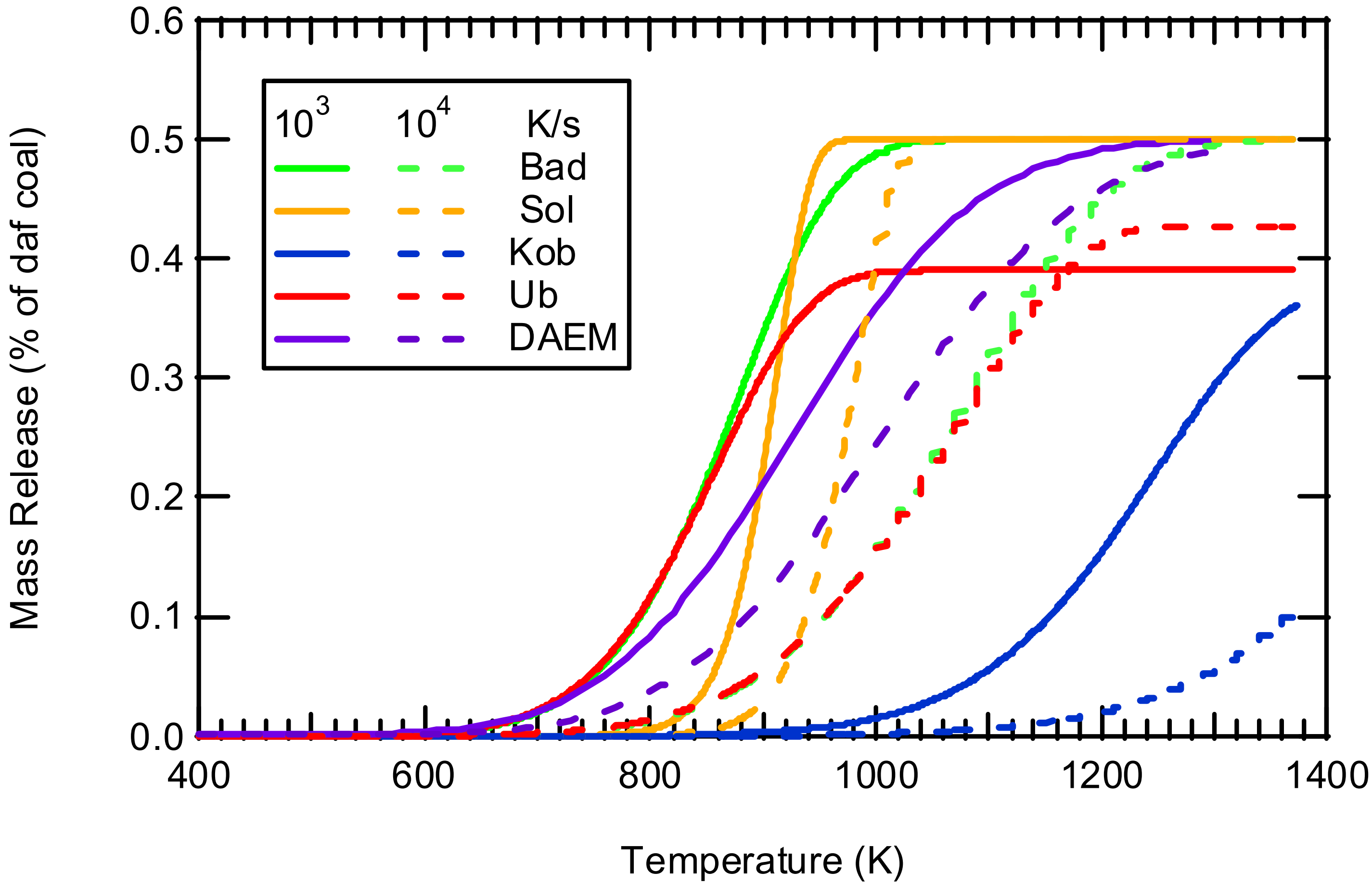


(10^4 K/s)



(10^3 K/s)

Effect of Heating Rate



Model Comparison

	# of constants	Yield = *f*(heating rate)?	Pressure effects?	T effect?	Coal type?
1-Step	A,E,V*			X	
2-step	A1,E1,Y1 A2,E2,Y2	x		X	
DAEM	A,E0,Sigm a,V*			X	

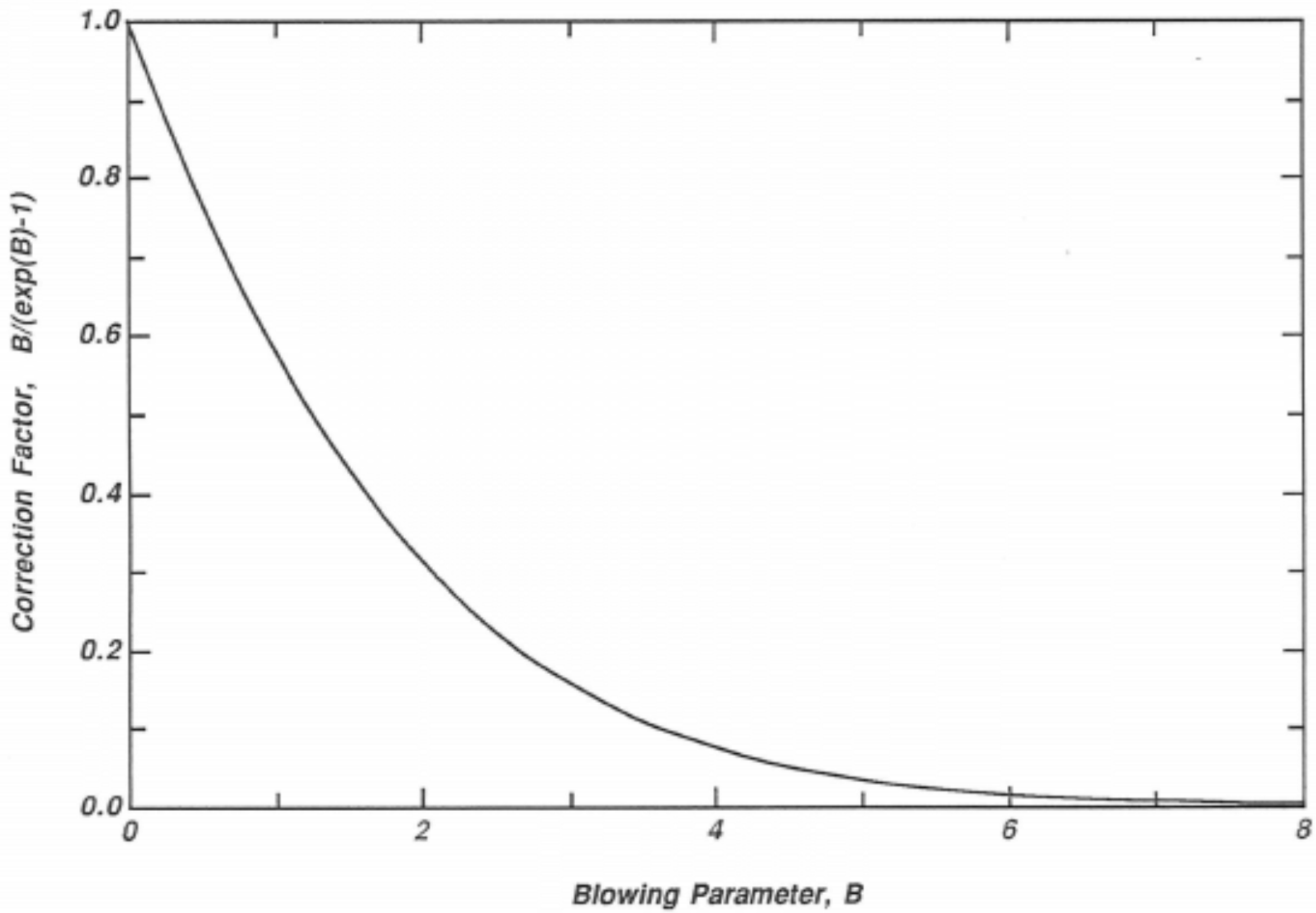
Industrial practice: Use 2-step,
Y_1 = ASTM volatiles yield,
$Y_2 = 2Y_1$

Result: works OK but not great

Blowing Factor

See MS Word Handout

Effect of the Blowing Factor



$$B = \frac{\left(-\frac{dm_p}{dt}\right) C_{p,g}}{2\,\pi\,d_p\,k_g}$$