SIMULATION OF COMPLEX MULTI-PHASE, MULTI-COMPONENT, REACTING FLOWS IN POROUS MEDIA

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Abstract

In this study we are concerned with the modelling of multi-component, multi-phase chemically reacting flows in porous media, with particular application to the spontaneous combustion of coal and the extraction of coalbed methane.

These two related problems involve complex multiphase, multi-component flow in a porous medium. Chemical reactions, adsorption, gaseous diffusion and changes in porosity and permeability are important in one or both of these problems. These matters are discussed in general in the first few chapters of the thesis.

Several models for the spontaneous combustion of coal that include the effect of a diminishing reaction rate are investigated and a new formulation in the form of a generic power law model is introduced.

A numerical module for modelling the spontaneous combustion of coal is described, based on the TOUGH2 code. A new equation of state (EOS) module is developed including realistic physical properties for all gases involved. The modified version of TOUGH2 is used for modelling the adiabatic method for testing the reactivity of coal samples. The results agree very well with experimental measurements for coal samples from different mines in New Zealand and Australia.

Moisture effect on the reaction rate was then introduced to TOUGH2 using a new two-phase EOS module with water and air broken into its main components (Nitrogen, Oxygen, Carbon dioxide and Argon).

Finally the production of methane from low rank coalbeds is investigated. A new EOS for mixture of water and methane is developed and incorporated into the TOUGH2 code to produce a new and versatile coalbed methane simulator. It is validated by running some simple test problems and comparing results with those obtained with the commercial COMET simulator.

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To My Homeland Iraq

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Nomenclature

Because of the extensive literature review and the many different applications discussed in this work, it is impossible to have a common notation throughout the thesis. The nomenclature given below includes the notation used throughout the work, while the other notation is defined differently as it appears in each chapter.

A	Area	m^2
A_0	Arrhenius pre-exponential factor (first order)	$1/s$
A_0'	Arrhenius pre-exponential factor for coal (Chapter 6)	$m^3/kg_{coal}\, s$
A_0''	Arrhenius pre-exponential factor (zero order)	$1/s$
Bi	Biot number $Bi = hx/K$	
C	Concentration	kg/m^3
Cp	Specific heat capacity	kJ/kgK
c_K	Cozeny's constant	
c	Compressibility	$1/Pa$
D	Diffusion coefficient	m^2/s
D_{th}	Thermal diffusivity $D_{th} = K/\rho Cp$	m^2/s
$d_\beta^{(\kappa)}$	Diffusion coefficient of phase β in component κ	m^2/s
d	Diameter	m
E_a	Activation energy	J/mol
F_f	Formation factor (Chapter 3)	
$\mathbf{F}^{(\kappa)}$	Flux of component κ	kg/m^2s or J/m^2s
$f^{(\kappa)}$	Mass fraction of component κ adsorbed per mass of solid	kg^{κ}/kg^{solid}

$\mathbf{g}$	Gravitational acceleration	m/s^2
$G_s^{(i)}$	Gas storage capacity of component i	m_g^3 / kg_{coal}
h	Heat transfer coefficient (convection)	W/m^2K
h	Cleat thickness (Chapter 8)	m
$H^{(\kappa)}$	Enthalpy of component κ	J/kg
h_{fg}	Latent heat of water	J/kg
$\boldsymbol{J}$	Jacobian matrix	
K	Thermal conductivity	$W/m\ K$
k	Permeability	$m^2\ (10^{-12}\ Darcy)$
K_d	Distribution coefficient	m^3/kg_{solid}
K_h	Henry's constant	$Pa\ (N/m^2)$
L	Length	m
L_e	Effective length	m
$M_\beta^{(\kappa)}$	Mass accumulation term of component κ in phase β	kg/m^3
M^{NK+1}	Heat accumulation term in multi-phase system	J/m^3
M_{AD}	Adsorbed mass accumulation term	kg/m^3
$MW^{(\kappa)}$	Molar weight of component κ	$kg/kmol$
n	Reaction order	
$\mathbf{n}$	Unit normal vector	
NK	Number of mass components	
NPH	Number of phases	
O_{ad}	Oxygen adsorbed on the coal surface	kg_{O_2}/kg_{coal}
$P^{(\kappa)}$	Partial pressure of component κ	$Pa\ (N/m^2)$
P	Pressure	$Pa\ (N/m^2)$
Q	Ionic activity product (Chapter 1)	
Q	Heat released by reaction (Exothermicity)	J/kg

$q^{(\kappa)}$	External sink/source of component κ	$kg/m^3\ s$ or $J/m^3\ s$
R	The universal gas constant (8.3145)	$kJ/kmol\ K$
R_t	Retardation factor (Chapter 4 and Chapter 8)	
Rf	Recovery factor (Chapter 8)	
R_{70}	Self-heating rate index (40 to 70 $^\circ C$) (Chapter 6)	$^\circ C/hour$
RH	Relative Humidity	
r	Radius	m
$r^{(\kappa)}$	Reaction rate of component κ	$kg/m^3\ s$
Re	Reynolds number	
S	Saturation	
SR	Stiffness ratio	
T	Temperature	$^\circ C$
T_K	Absolute Temperature	K
t	Time	$s\ (sec)$
t_{pr}	Prior reaction (oxidation) time (Chapter 5)	$s\ (sec)$
$\mathbf{U}$	The intrinsic velocity	m/s
u	Specific internal energy	J/kg
$\mathbf{V}$	Darcy's velocity (volume flux) ($\mathbf{V} = \phi.\mathbf{U}$)	m/s
V_n	Volume of grid element n	m^3
$X_\beta^{(\kappa)}$	Mass fraction of component κ in phase β	$kg_\beta^{(\kappa)}/kg_\beta^{(total)}$
x	Distance	m
$Z^{(\kappa)}$	Compressibility factor of component κ	
Γ_n	Surface area of grid element n	m^2
Γ	Gama function (Chapter 5)	
α	Molar weight ratio	
α	Empirical constant for the diminishing rate law (Chapter 5)	
α_L	Longitudinal dispersion coefficient	m^2/s

α_T	Transverse dispersion coefficient	m^2/s
∇	Gradient	
λ	Reaction rate coefficient	
λ	Non-isothermal reaction rate coefficient, $\lambda = A_0 \exp(-E_a/RT)$	
λ_0	Isothermal reaction rate coefficient, $\lambda_0 = A_0 \exp(-E_a/RT_0)$ (Chapter 5)	
ρ	Density	kg/m^3
v	Kinematic viscosity (μ/ρ)	m^2/s
μ	Dynamic viscosity	$N\ s/m^2$ ($Pa\ s$)
μ	Constant, $\mu = 1/\delta_0(1+\beta)$ (Chapter 5)	
υ	Reaction stoichiometric coefficient	
χ	Mole fraction	
β	Constant $\beta = Q/\rho Cp$ (Chapter 4)	
β	New empirical constant for the diminishing rate law (Chapter 5)	
δ_0	Modified Frank-Kamenetskii parameter (Chapter5) $\delta_0 = (E_a/RT_0^2)(QO_0 A_0 \tau/C_p)\exp(E_a/RT_0)$	
ε	Reduced ambient temperature, $\varepsilon = RT_0/E_a$ (Chapter 5)	
γ	Incomplete Gamma function (Chapter 5)	
ξ	Constant, $\xi = 1/v(1+b)$ (Chapter 5)	
ν	Constant, $\nu = \sigma/\varepsilon$ (Chapter 5)	
θ	Reduced excess temperature, $\theta = (T - T_0)E_a/RT_0^2$ (Chapter 5)	
σ	Constant, $\sigma = QO_0/CpT_0$ (Chapter 5)	
τ	Tortuosity ($\tau = L_e/L$) $\tau > 1$	
τ	Characteristic time scale ($\tau = t/t_{pr}$) (Chapter 5)	
τ	Sorption time (Chapter 8)	s (sec)
τ_f	Tortuosity factor ($\tau_f = \tau^2$)	
ϕ	Porosity	

Subscripts

ad	Adsorption
b	Bulk
$coal$	Coal
eff	Effective
eq	Equilibrium
f	Fluid
f	Fracture (Chapter8)
g	Gas
in	Insoluble mineral (Chapter2)
$\circ$	Initial state (initial condition)
L	Langmuir
l	Liquid
m	Mixture
m	Soluble mineral (Chapter2)
m	Matrix (Chapter 8)
p	Particle
r	Relative
s	Solid
s	Skin (Chapter8)
std	Standard conditions (101325 Pa and 288.6 K) (Chapter 8)
v	Vapor
β	Phase (gas or liquid)

Superscript

adv	Advective
air	Air
Ar	Argon
CH_4	Methane
CO_2	Carbon dioxide

dis	Diffusive (dispersive)
e	Equilibrium
N_2	Nitrogen
O_2	Oxygen
sat	Saturation conditions
κ	Component (mass or heat)
*	Non-dimensional form (Chapter5)

Abbreviations

BHP	Bottom hole pressure
CBM	Coalbed methane
DEA	differential-algebraic equations
ECBM	Enhanced coalbed methane
EOS	Equation of state
FHZ	Fastest heating zone
IFDM	Integrated finite difference method
MINC	Multiple interacting continua
NR	Newton-Raphson
ODE	Ordinary differential equation
PDE	Partial-differential equations
REV	Representative elementary volume
STP	Standard temperature and pressure (101325 Pa and 288.6 K)
TDS	Total dissolved solids