Mathematical/Numerical modeling on moisture evaporation, pyrolysis and smoldering of porous media

Sui-Hang YAN

DOCTOR OF PHILOSOPHY
City University of Hong Kong
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CITY UNIVERSITY OF HONG KONG

香港城市大學

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多孔物質的水份蒸發,高溫分解及陰燃的數學模型及數值模擬

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Sui-Hang YAN
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Abstract

"I was able to see further because I was standing on the shoulders of giants"

Sir Isaac Newton

A full procedure of numerical modeling on Moisture Evaporation, Pyrolysis and Smoldering (MEPS) of porous material has been extensively discussed. From the starting point on fundamental theories development on MEPS modeling, implementation on numerical techniques to the computational code realization, an in-depth discussion was illustrated in this thesis.

The effects of material physical and chemical structure, anisotropic characteristics, heat and mass transfer in porous media which affecting the behavior during evaporation, pyrolysis and smoldering are extensively reviewed.

A new mathematical model for evaporation, pyrolysis and smoldering of porous media which included sophisticated chemical and physical processes involved has been developed. The model comprises detailed considerations on fundamental multi-phase heat transfer (conductive, convective and radiative), momentum and mass transfer (evaporation, pyrolysis and smoldering).

It was found that the proposed model cannot be solved by standard Finite Volume method alone due to the complexity of proposed mathematical model. Some specific numerical modeling problems such as thermal non-equilibrium between phases, pressure coupling inside low permeability material, un-saturated moisture evaporation and high order chemical reactions need specific treatment. Several innovative methods

on tackling these problems were introduced. These treatments were found robust in solving modeling problems and without introduced much additional computational demand. Details of these methods were illustrated in thesis.

With the merits of those innovative techniques, the proposed model was solved successfully and implemented in a computational code which written in FORTRAN 90. The general procedures and the remark points utilized in the MEPS computational code are illustrated

The computational code was applied to predict the moisture evaporation and pyrolysis of wet wood. The results show that current model is superior in the prediction of mass loss rate and the surface temperature in different heating conditions. It demonstrated that the current model can be used to describe the sophisticated chemical and physical process. Meanwhile, a further modeling validation was undertaken on smoldering of polyurethane foam. The predicted temperature history during smoldering was found excellent agreement with the measured data. The phenomenon found in the experimental, included preheating, settling, front marching and quenching, are also captured by the present model.

A preliminary extension of the model for the simulation on autoignition, pilot ignition and flame spread is also discussion in the late section. These simulations involved the comprehensive solid-gas combustion. It demonstrated that the proposed model is capable on modeling solid-gas combustion which only some minor modifications are needed to be made on both equation set and numerical implementation. This possibility greatly reduces the computation effort on performing solid-gas combustion.

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Nomenclature

Symbols

a, b	*Coefficients of algebraic equation*
a, b, c	*Blending function*
d	*Pore diameter*
e	*Error vector*
f	*Mass fraction*
g	*Gravitational vector*
h	*Specific enthalpy*
h_c	*Convective heat transfer coefficient*
i, j, k	*Coordinate at the Cartesian coordinate*
k	*Conductivity*
n	*Normal vector*
m	*Phase change rate*
p	*Pressure*
q	*Heat flux*
r	*Position vector*
t	*Time*
u	*Diffusion velocity, x-component velocity*
v	*Velocity*
x, y, z	*Cartesian coordinate*
A	*Area, Pre-exponential factor*
C_p	*Specific heat capacity*
D	*Diffusive conductance*
E	*Activation Energy, Evaporation/Condensation coefficient*
F	*Forchheimer Tensor, Strength of convection*
I,J,K	*Maximum coordinate at Cartesian coordinate*
I	*Identity matrix*
J	*Flux term*
K	*Permeability Tensor*
L	*Latent Heat*
M	*Molecular Mass*
P	*Peclet no.*
Q	*Incident heat flux*
R	*Homogenous reaction, Universal gas constant, Mass residual*

S	*Source term*
T	*Temperature*
U_m	*Weighted mean velocity of different phase*
V	*Volume*
ε	*Porosity*
ρ	*Density*
σ	*Stefan-Boltzmann constant*
θ	*Mass transfer coefficient*
ω	*Interface velocity*
τ	*Shear force*
ν	*Stoichiometric ratio*
μ	*Dynamic viscosity*
χ	*Relaxation factor*
Λ	*Specific surface Area*
Γ	*Interfacial heat transfer coefficient*
Ξ, Ψ, Z	*Quantity of any order*
$\mathrm{H}, \Theta, \pi, o$	*Second order tensor*
Υ	*Mass diffusivity*
Φ	*Variable*

Subscripts

atm	*atmosphere*
amb	*ambient*
bd	*Boundary*
e,w,n,s,t,b	*Face location of Control volume*
eff	*Effective quantity*
i	*Summation of component i over same phase*
int	*Interface*
j	*Component j of single phase*
ref	*reference*
sat	*Saturation*
sur	*surface*
E,W,N,S,T,B,P	*Nodal point of control volume*
∞	*Far field*
v	*vapor*
α	*Solid Phase*
β	*Liquid Phase*

γ	*Gas Phase*
ϕ	*Any phase*
$\alpha\beta$	*Connection of solid-liquid phases*
$\beta\gamma$	*Connection of liquid-gas phases*
$\gamma\alpha$	*Connection of gas-solid phases*

Superscripts

$\sim$	*Variation*
$_$	*Interpolated value, mean value*
$\cdot$	*Rate of change*
n	n^{th} *iteration*
m	m^{th} *iteration*
o	*Old value*
I,II	*Indicator*
α	*Solid Phase*
β	*Liquid Phase*
γ	*Gas Phase*
ϕ	*Any phase*
$\alpha\beta$	*Connection of solid-liquid phases*
$\beta\gamma$	*Connection of liquid-gas phases*
$\gamma\alpha$	*Connection of gas-solid phases*

Operator

$<>$	*Superficial averaging*
$<>_\alpha$	*Intrinsic solid phase average*
$<>_\beta$	*Intrinsic liquid phase average*
$<>_\gamma$	*Intrinsic gas phase average*
∇	*Divergence*
$\bullet$	*Dot product*
$>>$	*Much large than*
Δ	*Increment*
$\approx$	*approximate*
$\lvert\ \rvert$	*Absolute value*

Abbreviations

2-D	*Two-Dimensional*
3-D	*Three-Dimensional*
Bi-CG	*Bi-Conjugate Gradient Method*
Bi-CGSTAB	*Bi-Conjugate Gradient Stabilized Methods*
CDS	*Central Differencing Scheme*
CFD	*Computational Fluid Dynamics*
CG	*Conjugate Gradient Method*
CGS	*Conjugate Gradient Squared Method*
CV	*Control Volume*
MEPS	*Moisture Evaporation, Pyrolysis and Smoldering*
ES	*Exponential Scheme*
FDM	*Finite Differencing Method*
FEM	*Finite Element Method*
FVM	*Finite Volume Method*
GA	*Genetic Algorithm*
MSIP	*Modified Strongly Implicit Procedure*
MSIMPLER	*Modified Semi-Implicit method for Pressure - Linked Equation Revised*
NS	*Navier-Stokes Equation*
ODE	*Ordinary Differential Equation*
PDE	*Partial Differential Equation*
PLS	*Power Law Scheme*
PMMA	*Polymethyl methacrylate*
PU	*Polyurethane*
QUDS	*Quadratic Upwind Differencing Scheme*
QUICK	*Quadratic Upstream Interpolation for Convective Kinetics*
REV	*Representative Elementary Volume*
RH	*Relative Humidity*
RMS	*Root Mean Square*
SemiIP	*Semi-Implicit Procedure*
SIP	*Strongly Implicit Procedure*
SIMPLE	*Semi-Implicit method for Pressure - Linked Equation*
SIMPLEC	*Semi-Implicit method for Pressure - Linked Equation Consistent*
SIMPLER	*Semi-Implicit method for Pressure - Linked Equation Revised*

STARS	*Semi Time Accurate Reaction Scheme*
SUDS	*Skew Upwind Differencing Scheme*
TC	*Thermocouple*
TDMA	*Tri- Diagonal–Matrix Algorithm*
TFI	*Transfinite Interpolation Methods*
UDS	*Upwind Differencing Scheme*