Gpyro Workbook on Pyrolysis & Smouldering Problems

(Based on Version 0.8175)

https://doi.org/10.5281/zenodo.1212540

by

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(Revision Log)

Ver. No.	When	What	Who
	10/2014	Example problems selected	X.Huang and G.Rein
0.1	03/2018	Demo version released	H.Yuan and G.Rein

Contents

Gpyro is a powerful open-source simulation tool for computational study of pyrolysis and smouldering. As the creator and on-going developer, Christopher Lautenberger has published technical reference[1] and user's guidance[2] to help the users get started. Besides, as additional supporting documents, several sample cases have also been included in the installation package.

Nevertheless, due to the large number of input parameters and high degree of flexibility in specifying them, some beginning learners may still have difficulty in using this tool well, especially when applying it to investigate a specific case.

We therefore produce this document, aiming to further help Gpyro users. We adapt published researches to several typical solid pyrolysis/smouldering problems and demonstrate how to use Gpyro to solve these problems. In the solutions, the key setting steps and validated simulation results are shown along with some input files attached as reference. We hope this document can serve as a complementary document to the official user-supporting files (ie. technical reference and user's guidance) and provide more details for the implementation of Gpyro. Since it is a complementary rather than an overall user's guidance, before reading this document, users should first read through technical reference and user's guidance to get familiar with the basics on concepts, physical models, and implementation of Gpyro.

1 Difference between Version 0.700 and Version 0.8175

Although Gpyro is keeping updated, some users prefer to use the old version However, the first public version of Gpyro (V0.700) was released in 2009. During the past 9 years, Gpyro has been updated for more than 500 times and many new features (i.e 3D simulation, a more concise input interface and a better solver) have been added into the new version.

To make full use of this powerful tool, researchers are strongly recommended to transition from old versions to the new one. For helping old version users transition, important differences in input parameters, input interface and working mechanisms between Version 0.700 and version 0.8175 (the latest version) are therefore first disccused in this document.

1.1 GENERAL (General settings)

Compared to V0.700, the latest version has changed some entries in the **GENERAL** Worksheet. Five entries no longer exist in the V0.8175: SOLVE_POROSITY, PROPERTY_LINTERP, GAS_DIFFUSION, FRONT_GAS_DIFFUSION, MINIMUM_CONDUCTIVITY. On the other hand, some new entries are added.

For example, in V0.8175, we can specify different relaxation parameters to different variables. This is more flexible than the older version, which only allows for the setting of GLOBAL relaxation parameter. By tuning the relaxation separately to different parameters, converge might be easier to reach.

Other newly added parameters can be checked through the ***updating*** recordings http://reaxengineering.com/trac/gpyro/timeline?from=03%2F09%2F18&daysback=90&authors=&changeset=on&update=Update.

1.2 OUTPUT (Output)

In the OUTPUT Worksheet, the V0.8175 doesn't provide the entries of DUMP_ENERGY_BALANCE, DUMP_EVERYTHING anymore, but it adds two entries: the setting of IMESH index and the coordinate setting of y-axis (T), expanding the output to 3D. IMESH is the index of the mesh used for output. When IMESH=0, all meshes specified in GEOM worksheet will be output.

r	Quantity	index	IMESH	z (m)	x (m)	y (m)
1	MLR	0	0	0.0000	0.0000	0.0000
2	M/M0	0	0	0.0000	0.0000	0.0000
3	YI	1	0	0.0000	0.0000	0.0000
4	YI	2	0	0.0000	0.0000	0.0000
5	YI	3	0	0.0000	0.0000	0.0000
6	REACTION_RATE_K	1	0	0.0000	0.0000	0.0000
7	REACTION_RATE_K	2	0	0.0000	0.0000	0.0000
8	N_ITERATIONS	0	0	0.0000	0.0000	0.0000

Figure 1-1 OUTPUT worksheet in V0.8175

1.3 SPROPS (Condensed phase species properties)

No significant change is made in this worksheet, except for expanding the entry for setting the property heterogeneity from Z direction to z, x, y direction.

1.4 RXNS (Condensed phase reactions)

No difference at all. It should be noted that T_{crit} cannot be set through Excel worksheets different. If you want to use this parameter in the simulation, you should add this parameter manually in the .data file that produced from Excel worksheets.

1.5 GPROPS (Gas phase species properties)

The most significant change in GPROPS Worksheet is that the entry for specifying the initial fraction of gas species doesn't exist anymore. **This information is left to be specified in the IC Worksheet in V0.8175.**

1.6 GYIELDS (Gaseous yields matrix)

No difference at all

1.7 HGRXNS & GYIELDS (Gas-phase reactions & gaseous yields matrix)

No difference at all

1.8 IC (Initial conditions)

The **IC** worksheet plays a similar role as the **LAYERS** worksheet does in the Version 0.700, but with a more concise and clear interface.

IC #	T_0 (K)	T_{g0} (K)	P_0 (Pa)	$Y_{i0,1}$ (-)	$Y_{i0,2}$ (-)	$Y_{i0,3}$ (-)	$Y_{j0,1}$ (-)
1	300.0	300.0	101300.0	1.000	0.000	0.000	1.000

Figure 1-2 Initial conditions(IC) Worksheet in V0.8175

1.9 GEOM&BC (Geometry & Boundary Conditions)

In new version, these two worksheets differ the most from the old version. It change the way to specify boundary condition.

1.9.1 GEOM (Geometry)

This worksheet did not exist in the old version. However, in V.0.8175, since 3D simulation feature is added, a separate worksheet for setting geometry condition and mesh is necessary.

2	NMESH	Number of gpyro meshes										
1	NOBST	Number of OBST's										
	Mesh 01	Mesh 02	Mesh 03	Mesh 04	Mesh 05	Mesh 06	Mesh 07	Mesh 08	Mesh 09	Mesh 10	Mesh 11	Mesh 12
ZDIM	0.005	0.005										
NCELLZ	51	51										
XDIM	1	1										
NCELLX	1	1										
YDIM	1	1										
NCELLY	1	1										
GEOMETRY_FILE	'null'	'null'										
DEFAULT_SURF_IDX(1)	0	0										
DEFAULT_SURF_IDX(2)	0	0										
DEFAULT_SURF_IDX(3)	0	0										
DEFAULT_SURF_IDX(4)	0	0										
DEFAULT_SURF_IDX(5)	1	2										
DEFAULT_SURF_IDX(6)	3	3										
DEFAULT_IC	1	2										
OFFSETZ	0	0										
OFFSETX	0	0										
OFFSETY	0	0										
Enter obst information below:												
OBST #	Mesh #	z_1 (m)	z_2 (m)	x_1 (m)	x_2 (m)	y_1 (m)	y_2 (m)	IC #	SURF_IDX(1)	SURF_IDX(2)	SURF_IDX(3)	SURF_IDX(4)
1	1	0.000	0.005	0.000	1.000	0.000	1.000	1	0	0	0	0
2	2	0.000	0.005	0.000	1.000	0.000	1.000	2	0	0	0	0
3												
4												
5												
6												
7												
8												
9												
10												

Figure 1-3 GEOM worksheet in V0.8175

Figure 1-3 is the screen shot of GEOM worksheet.

ZDIM(XDIM/YDIM) and NCELLZ(NCELLX/ NCELLY) represents length(m) and number of cell.

SURF_IDX (N) is the index string used for transfering the boundary conditions specified in BC worksheet into GEOM worksheet. More specifically:

DEFAULT_SURF_IDX(1) corresponds to the -x direction;

DEFAULT_SURF_IDX (2) corresponds to the +x direction;

DEFAULT_SURF_IDX (3) corresponds to the -y direction;

DEFAULT_SURF_IDX (4) corresponds to the +y direction;

DEFAULT_SURF_IDX 5) corresponds to the -z direction;

DEFAULT_SURF_IDX (6) corresponds to the +z direction.

Literally, OBST means obstruction. It is used when simulating multi-layer case. More explanation for OBST can be found in [3]

1.9.2 BC (Boundary conditions)

As mentioned before, in V0.8175 **BC** worksheet doesn't include geometry information anymore. Boundary conditions are specified and then transferred to GEOM worksheet through the index of SURF_IDX.

To illustrate how this works, we can take the screenshots shown in Figure 1-3 and Figure 1-4 as an example. A boundary condition is specified with SURF_IDX set to 1 in Figure 1-4. Then the boundary condition is transferred to **GEOM** worksheet by setting "1" in the entry of DEFAULT_SURF_IDX(5)(SURF_IDX(5)) (Shown in Figure 1-3). This setting means that the No.1 boundary condition set in **BC** Worksheet is used as the boundary condition at -z direction, i.e top surface boundary condition.

			Solid Energy						Gas momentum		Gas energy			
	SURF_IDX	t (s)	q_e (W/m^2)	h_c (W/m^2-K)	~~ε_{bc}~~ (-)	T_∞ (K)	Reradiation	Fixed T (K)	m" (g/m^2-s)	P (Pa)	q_e (W/m^2)	h_c (W/m^2-K)	T_∞ (K)	Fixed T (K)
0	1	0	0	10	0	300	.FALSE.	-1	0	101300	0	12	300	-1000
1														

Figure 1-4 BC Worksheet in V0.8175

1.10 CASES (Batch mode calculation settings)

The **CASES** worksheet plays the same role as **QE** Worksheet does in V0.700, but with a far more concise interface. Only 5 entries are required to be set right now. All of the other entries existed in the

old version should be specified in the worksheet of **IC, GEMO** and **BC** and transferred through the index of **IMESH** to **CASES** worksheet.

2 Problem I: TGA Pyrolysis

The beginning users of Gpyro are strongly recommended to start from the simplest problem—0D pyrolysis problem. The problem we propose here is abstracted from the work conducted by Rein, Lautenberger [4]. More detailed description of the problem can be found in the original paper.

2.1 Problem Statement

A TGA experiment of polyurethane foam pyrolysis is carried out in nitrogen atmosphere. In the experiment, initial temperature is 300K and the heating rate is 20°C/min. Can you use Gpyro to reproduce this experiment and simulate how the reaction rates, mass loss rate and dimensionless weight of solid mass changes with temperature?

The kinetic scheme and parameters of foam pyrolysis are listed as below

$$\text{foam} \rightarrow \nu_{\beta,\text{p}}\beta\text{-foam} + \nu_{\text{g,p}}\text{gas} \tag{2-1}$$

$$\beta\text{-foam} \rightarrow \nu_{\text{c,p}\beta}\text{char} + \nu_{\text{g,p}\beta}\text{gas} \tag{2-2}$$

The reaction rate is assumed to have an Arrhenius form as follow[4]:

$$\dot{\omega}_i = A_i e^{-E_i/RT} m_i^{n_i} \tag{2-3}$$

Table 2-1 kinetic parameters for TGA pyrolysis problem[4]

Parameter	Value	Units
E_p	148	kJ/mol
$\log_{10}(A_p)$	11.3	$\log_{10}(1/s)$
n_p	0.21	–
$\nu_{\beta,p}$	0.70	kg/kg
$E_{p\beta}$	124	kJ/mol
$\log_{10}(A_{p\beta})$	8.2	$\log_{10}(1/s)$
$n_{p\beta}$	1.14	–
$\nu_{c,p\beta}$	0.05	kg/kg

2.2 Gpyro setting

2.2.1 SPROPS worksheet (Condensed phase species properties)

In TGA model, almost all of condensed phase species properties are not be used in the simulation, since condensed phase energy conservation equation[1] is simple as

$$T_s = T_{0s} + \beta t \tag{2-4}$$

, which is irrelevant to condensed phase properties. Thus, all of the property parameters can be specified arbitrarily.

However, there is an exception—density. Although density does not appear in the energy conservation equation either, it is relevant to the setting of stoichiometry in Gpyro. **In fact, Gpyro provides no place for us to specify stoichiometry directly. If stoichiometry is required to specify in the simulation, it can only be specified through density using the following equation (The detailed explanation of this equation can be found in** [1]**):**

$$\mathrm{SF}_k = 1 + \left(\frac{\rho_{B_k}}{\rho_{A_k}} - 1 \right) \chi_k \tag{2-5}$$

Since the absolute value of density is not important in 0D simulation, we can first set the bulk density of foam to 1000 kg/m^3 and the density of β-foam and char can be specified accordingly by taking the stoichiometry listed in Table 2-1 into equation (2-5), where χ_k should be set to 1 which means no volume change occurs during the reaction process. The final setting is shown in Figure 2-1.

ISPEC	Name	k_{0z} (W/m-K)	n_{kz} (-)	ρ_0 (kg/m^3)
1	foam	0.200	0.000	1000
2	belta_foam	0.200	0.000	700
3	char	0.200	0.000	35

Figure 2-1 The setting of densities for TGA pyrolysis problem

2.2.2 RXNS worksheet (Condensed phase reactions)

Apart from stoichiometry, all of other kinetic parameters shown in Table 2-1 should be specified in **RXNS** Worksheet as follow:

2	nrxns	# of reactions													
Specify reactions below. If 'To' species is not the name of a species specified in the 'props' worksheet, it is assumed to be gaseous															
IRXN	From (species A)	To (species B)	Z (s^{-1})	E (kJ/mol)	ΔH_s (J/kg)	ΔH_v (J/kg)	χ (-)	n (-)	n_{O2} (-)	$i_{kinetic\ model}$	$i_{O2\ rxn}$	m (-)	K_{cat} (-)	i_{cat}	T_{crit} (K)
1	foam	belta_foam	2.00E+11	148	0.00E+00	0.00E+00	1	0.21	0	0	0	0	0	0	0
2	belta_foam	char	1.58E+08	124	0.00E+00	0.00E+00	1	1.14	0	0	0	0	0	0	0

Figure 2-2 The setting of RNXS worksheet for TGA Pyrolysis problem

Note that Gpyro uses an unconventional treatment of conservation rate in the expression of reaction rate[1]. However, in the 0D pyrolysis problem proposed here, the reaction rate is still written in the conventional form. Thus, we have to make the transformation of reaction treatment by setting "**CONVENTIONAL_RXN_ORDER**", an input entry in **GENERAL** Worksheet, as "TRUE".

2.2.3 GpyroS worksheet (Gas phase species properties)

Both the gas species consisting the atmosphere and the gas species produced in chemical reactions should be specified in the Worksheet of **GPROPS**.

However, in this 0D problem, gas properties are also irrelevant to the simulation results and thus they can be specified arbitrarily.

3	NGSPEC	# of gaseous species				
1	IBG	Species index of background gaseous species (for calculating diffusivity)				
2	IO2	Species index of oxygen				
1000	CPG	Specific heat capacity of gas (J/kg-K)				
IGSPEC	Name	M (g/mol)	σ (Å)	ε/k (K)	~~c_{p0} (J/kg-K)~~	~~n_c (-)~~
1	pyrolysate	44	5.061	254	~~1000~~	~~0.00~~
2	oxygen	32	5.061	254	~~1000~~	~~0.00~~
3	nitrogen	28	5.061	254	~~1000~~	~~0.00~~

Figure 2-3 The setting of GPROPS Worksheet for TGA pyrolysis problem

2.2.4 GYIELDS worksheet (Gas yields matrix)

Gas yield matrix is the concept proposed by Lautenberger in developing Gpyro. Its defination can be found in [1]. **The principle of setting in GYIELDS Worksheet is that the sum of every activated reaction column should be equal to 1**.

3	NGSPEC	# of gaseous species	
		Reaction number ->	
		1	2
	From	foam	belta_foam
	To	belta_foam	char
	Z	2.00E+11	1.58E+08
	E	148.0	124.0
	ΔH_s	0.00E+00	0.00E+00
	ΔH_v	0.00E+00	0.00E+00
	χ	1.00	1.00
	n	0.21	1.14
	n_{O2}	0.00	0.00
		Yields matrix:	
		Reaction number ->	
IGSPEC	Name	1	2
1	pyrolysate	1.00	1.00
2	oxygen	0.00	0.00
3	nitrogen	0.00	0.00
4	0	0.00	0.00
5	0	0.00	0.00
6	0	0.00	0.00
7	0	0.00	0.00
8	0	0.00	0.00
9	0	0.00	0.00
10	0	0.00	0.00
	TOTALS:	1.00	1.00

Figure 2-4 The setting of **GYIELDS** Worksheet for TGA pyrolysis problem

2.2.5 IC worksheet (Initial conditions)

As illustrated in section 1.8, one of the most significant change in input interface is initial conditions. In the **IC** worksheet, we can set initial temperature, pressure and mass fraction. Note that i and j represents condensed and gas phase respectively **and the index number of species correspond to their numbering in the worksheet of SPROPS and GPROPS.**

IC #	T_0 (K)	T_{g0} (K)	P_0 (Pa)	$Y_{i0,1}$ (-)	$Y_{i0,2}$ (-)	$Y_{i0,3}$ (-)	$Y_{j0,1}$ (-)	$Y_{j0,2}$ (-)	$Y_{j0,3}$ (-)
1	300.0	300.0	101300.0	1.000	0.000	0.000	0.000	0.000	1.000

Figure 2-5 The setting of **IC** worksheet for TGA pyrolysis problem

2.2.6 GEOM and BC worksheet (Geometry and boundary conditions)

In 0D simulation, GEOM worksheet and BC worksheet are not used and they can be left as the default setting.

2.2.7 CASES worksheet (Batch mode setting)

The **CASES** worksheet is where the heating rate (β) should be set. For 0D simulation, "**0D?**" should be set as "**TRUE**".

1	Number of cases to run			
Case #	IMESH	t_{stop} [s]	0D?	β [K/min]
1	1	1800	.TRUE.	20.0

Figure 2-6 The setting of **CASES** worksheet for TGA pyrolysis problem

2.3 Simulation results

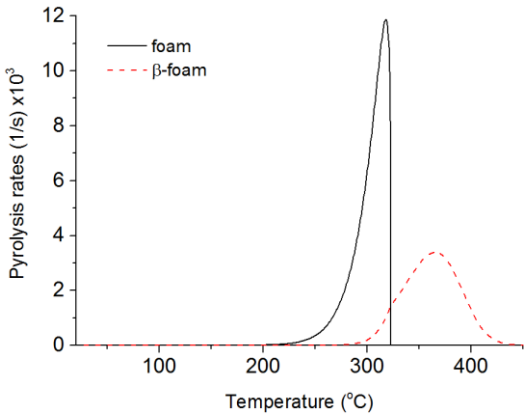

Figure 2-7 Pyrolysis rate as a function of temperature

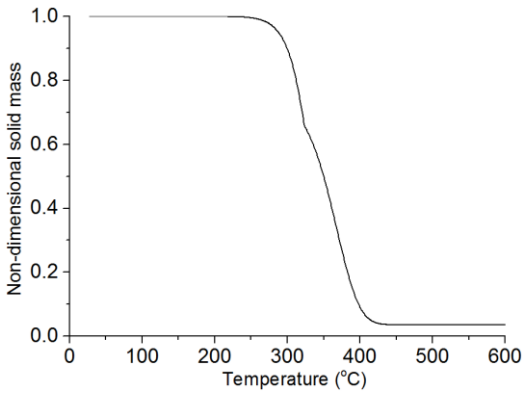

Figure 2-8 Solid mass as a function of temperature

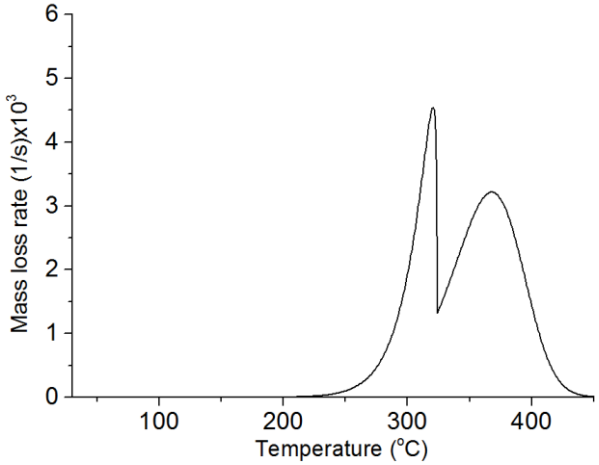

Figure 2-9 Mass loss rate as a function of temperature

Figure 2-7, Figure 2-8, Figure 2-9 are the simulation results obtained by V0.8175. These results match well with the original work[4]. It should be noted that the reaction rate defined in Gpyro is a volumetric term, which is different from the conventional definition of reaction rate. If we want to plot the conventional reaction rate in the figure (as shown in Figure 2-7), we need convert the volumetric term into the conventional term. (A detailed discussion of this issue can be found in Gpyro Google https://groups.google.com/forum/#!topic/gpyro-working-group/ZYWUzymejeY)

3 Problem II: TGA Smouldering

The TGA smouldering problem is also abstracted from [4]. It is more complicated than the pyrolysis problem since oxidation is taken into account.

3.1 Problem Statement

A TGA experiment of polyurethane foam pyrolysis is carried out in air atmosphere (Y_{O2}=0.23，Y_{N2}=0.77). In the experiment, initial temperature is 300K and the heating rate is 20°C/min. Can you use Gpyro to predict how reaction rates, mass loss rate and dimensionless weight of solid mass change with temperature?

The kinetic scheme and parameters of foam smouldering is listed as below

$$\text{foam} \rightarrow \nu_{\beta,\text{p}}\beta\text{-foam} + \nu_{\text{g,p}}\text{gas} \tag{3-1}$$

$$\beta\text{-foam} \rightarrow \nu_{\text{c,p}\beta}\text{char} + \nu_{\text{g,p}\beta}\text{gas} \tag{3-2}$$

$$\text{foam} + \nu_{\text{O}_2,\text{o}}\text{O}_2 \rightarrow \nu_{\text{c,o}}\text{char} + \nu_{\text{g,o}}\text{gas} \tag{3-3}$$

$$\beta\text{-foam} + \nu_{\text{O}_2,\text{o}\beta}\text{O}_2 \rightarrow \nu_{\text{c,o}\beta}\text{char} + \nu_{\text{g,o}\beta}\text{gas} \tag{3-4}$$

$$\text{char} + \nu_{\text{O}_2,\text{c}}\text{O}_2 \rightarrow \nu_{\text{r,c}}\text{residue} + \nu_{\text{g,c}}\text{gas} \tag{3-5}$$

The reaction rate is assumed to have an Arrhenius-type shown as below:

$$\dot{\omega}_i = A_1 e^{-E_i/RT} m_i^{n_i} y_{\text{O}_2}^{\delta} \tag{3-6}$$

Table 3-1 kinetic parameters for TGA smouldering problem [4]

Parameter	Value	Units
E_p	148	kJ/mol
$\log_{10}(A_p)$	11.3	$\log_{10}(1/s)$
n_p	0.21	–
$\nu_{\beta,p}$	0.70	kg/kg
$E_{p\beta}$	124	kJ/mol
$\log_{10}(A_{p\beta})$	8.2	$\log_{10}(1/s)$
$n_{p\beta}$	1.14	–
$\nu_{c,p\beta}$	0.05	kg/kg
E_o	194	kJ/mol
$\log_{10}(A_o)$	15.4	$\log_{10}(1/s)$
n_o	0.52	–
$\nu_{c,o}$	0.57	kg/kg
$E_{o\beta}$	194	kJ/mol
$\log_{10}(A_{o\beta})$	15.4	$\log_{10}(1/s)$
$n_{o\beta}$	0.52	–
$\nu_{c,o\beta}$	0.57	kg/kg
E_c	201	kJ/mol
$\log_{10}(A_c)$	15.2	$\log_{10}(1/s)$
n_c	1.23	–
$\nu_{r,c}$	0.23	kg/kg

3.2 Gpyro setting

3.2.1 SPROPS worksheet (Condensed phase species properties)

As illustrated in section 2.2.1, for a 0D problem what really needs to set in **SPROPS** worksheet is just density.

However, as oxidation is involved in the smouldering problem, the simulation becomes more complicated than the pyrolysis problem. As mentioned in section 2.2.1 , density should be specified according to stoichiometry. However, when an identical species are generated from different reaction paths with variant stoichiometry the problem comes: there would be multiple rather than one density corresponding to an identical species, but Gpyro does not permit an identical species to be specified with different densities.

Our solution to this problem is to split the identical species into different species with different name and density, but in analysis we regard them as a whole part and sum their values up when needed.

In this specific case, char is generated from three different paths (reaction (3-2)、(3-3)、(3-4)) which lead to 3 different densities. Thus, in Gpyro, we split char into 3 different species for each

reaction path. Moreover, since char is the intermediate species, the splitting of char also leads to the splitting of residue, which is the final product in this problem. Thus, to simulate this problem in Gpyro, we need to set 8 rather than 4 species. The setting of SPORPS section is listed below:

ISPEC	Name	k_{0z} (W/m-K)	n_{kz} (-)	ρ_0 (kg/m^3)
1	foam	0.200	0.000	1000
2	belta_foam	0.200	0.000	700
3	pbelta_char	0.200	0.000	35
4	o_char	0.200	0.000	570
5	obelta_char	0.200	0.000	399
6	pbelta_residue	0.200	0.000	8.05
7	o_residue	0.200	0.000	131.1
8	obelta_residue	0.200	0.000	91.77

Figure 3-1 The setting of SPROPS worksheet for TGA smouldering problem

3.2.2 RXNS worksheet (Condensed phase reactions)

The reaction scheme for condensed phase reactions is a 5-step scheme as shown in worksheet 3.1. However, the number of reactions we should set in **RXNS** is 7 rather than 5. It is because we split char into three different species and thus we also need three different reactions to consume it. The setting of RXNS worksheet is shown in Figure 3-2. **Note that according to the form of oxidation reaction rate (**(3-6)**) used in this problem,** the value of I_{O2} should be specified to 1.

7	nrxns	# of reactions													
Specify reactions below. If 'To' species is not the name of a species specified in the 'props' worksheet, it is assumed to be gaseous															
IRXN	From (species A)	To (species B)	Z (s^{-1})	E (kJ/mol)	ΔH_s (J/kg)	ΔH_v (J/kg)	χ (-)	n (-)	n_{O2} (-)	$i_{kinetic\ mode}$	i_{O2} rxn	m (-)	K_{cat} (-)	i_{cat}	T_{crit} (K)
1	foam	belta_foam	2.00E+11	148	0.00E+00	1.00E+06	1	0.21	0	0	0	0	0	0	0
2	belta_foam	pbelta_char	1.58E+08	124	0.00E+00	1.00E+06	1	1.14	0	0	0	0	0	0	0
3	foam	o_char	2.51E+15	194	0.00E+00	1.00E+06	1	0.52	1	0	1	0	0	0	0
4	belta_foam	obelta_char	2.51E+15	194	0.00E+00	1.00E+06	1	0.52	1	0	1	0	0	0	0
5	pbelta_char	pbelta_residue	1.58E+15	201.00	0.00E+00	1.00E+06	1	1.23	1	0	1	0	0	0	0
6	o_char	o_residue	1.58E+15	201.00	0.00E+00	1.00E+06	1	1.23	1	0	1	0	0	0	0
7	obelta_char	obelta_residue	1.58E+15	201.00	0.00E+00	1.00E+06	1	1.23	1	0	1	0	0	0	0

Figure 3-2 The setting of RXNS Worksheet for TGA smouldering problem

3.2.3 GpyroS worksheet (Gas phase species properties)

Since gas properties have nearly no influence on the 0D simulation, the gas phase species properties setting is not important in the simulation.

1	3	NGSPEC	# of gaseous species					
2	1	IBG	Species index of background gaseous species (for calculating diffusivity)					
3	2	IO2	Species index of oxygen					
4	1000	CPG	Specific heat capacity of gas (J/kg-K)					
5								
6	IGSPEC	Name	M (g/mol)	σ (Å)	ε/k (K)	~~c_{p0} (J/kg-K)~~	~~n_c (-)~~	
7	1	pyrolysate	44	5.061	254	~~1000~~	~~0.00~~	
8	2	oxygen	32	5.061	254	~~1000~~	~~0.00~~	
9	3	nitrogen	28	5.061	254	~~1000~~	~~0.00~~	

Figure 3-3 The setting of GPROPS worksheet for TGA smouldering problem

3.2.4 GYIELDS worksheet (Gas yields matrix)

For 0D simulation, the gas yields factor for the consumption of oxidation and production of pyrolysate can be specified arbitrarily as long as the sum of each column equals to 1.

IGSPEC	Name	1	2	3	4	5	6	7
1	pyrolysate	1.00	1.00	2.00	2.00	2.00	2.00	2.00
2	oxygen	0.00	0.00	-1.00	-1.00	-1.00	-1.00	-1.00
3	nitrogen	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	TOTALS:	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Figure 3-4 The setting of GYIELDS worksheet for TGA smouldering problem

3.2.5 IC worksheet (Initial conditions)

The initial condition is set as below.

1	NIC	Number of initial conditions groups to apply												
Enter layer information below:														
IC #	T_0 (K)	T_{g0} (K)	P_0 (Pa)	$Y_{i0,1}$ (-)	$Y_{i0,2}$ (-)	$Y_{i0,3}$ (-)	$Y_{i0,4}$ (-)	$Y_{i0,5}$ (-)	$Y_{i0,6}$ (-)	$Y_{i0,7}$ (-)	$Y_{i0,8}$ (-)	$Y_{j0,1}$ (-)	$Y_{j0,2}$ (-)	$Y_{j0,2}$ (-)
1	300.0	300.0	101300.0	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.230	0.770

Figure 3-5 The setting of IC worksheet for TGA smouldering problem

3.2.6 GEOM and BC worksheet (Geometry and boundary conditions)

In 0D simulation, GEOM worksheet and BC worksheet are not used and they can be left as the default setting.

3.2.7 CASES worksheet (Batch mode setting)

The setting in CASES worksheet is identical to that shown in section **Error! Reference source ot found.**.

3.3 Simulation results

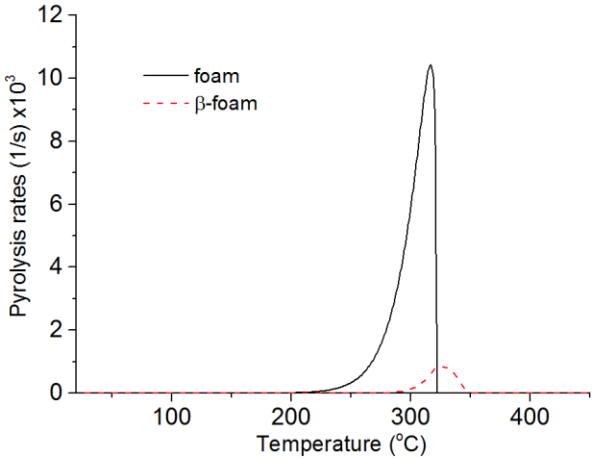

Figure 3-6 pyrolysis rate as a function of temperature

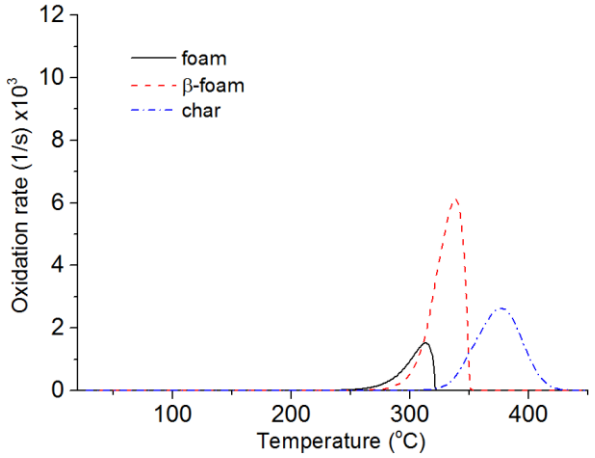

Figure 3-7 Oxidation rate as a function of temperature

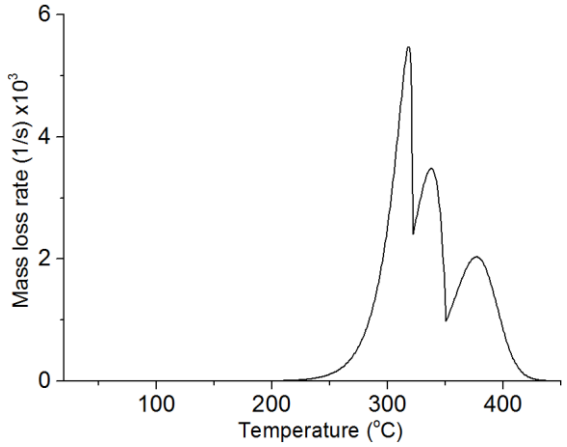

Figure 3-8 Mass loss rate as a function of temperature

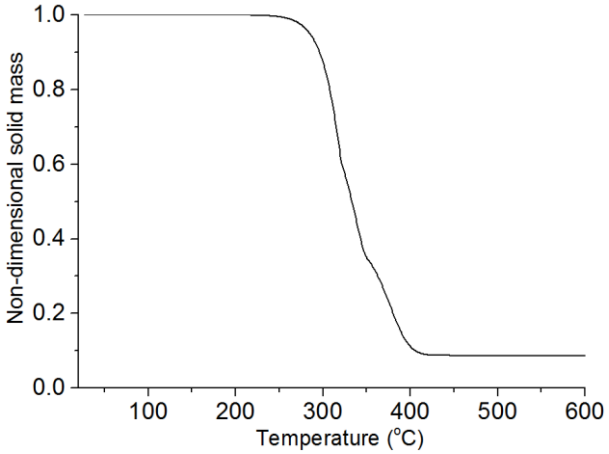

Figure 3-9 Non-dimensional mass loss as a function of temperature

The simulation solution to the 0D smouldering problem is displayed above. It should be noted that the oxidation rate curve of char is plotted by summing up the oxidation rates of three "types" of char. The simulation results also match well with the original work[4].

4 Problem III: 1D pyrolysis

In 1982, Kashiwagi and Ohlemiller [5] conducted an experiment to investigate the non-flaming gasification of PMMA. In the experiment, A PMMA sample (40mm×40mm square with a 15mm thickness) was exposed to different levels of irradiation in different gas atmospheres. The surface temperature and weight of sample were monitored to investigate the characteristics of PMMA gasification. In 2009, Lautenberger and Fernandez-Pello [6] simulated this experiment using Gpyro.

The 1D pyrolysis problem proposed here is adapted from their research.

4.1 Problem Statement

A PMMA sample (40mm×40mm square with a 15mm thickness) is irradiated at a rate of 40 kW/m^2 in nitrogen atmosphere. The initial temperature for both the ambient and sample is 300K. The natural convection on both top and bottom boundary is considered and the natural convective heat transfer coefficient is assumed to be 10W/m^2-K. Figure 4-1 is the schematic illustration of this problem. Can you use Gpyro to simulate this experiment and predict how temperature profile, mass loss rate varies with time.

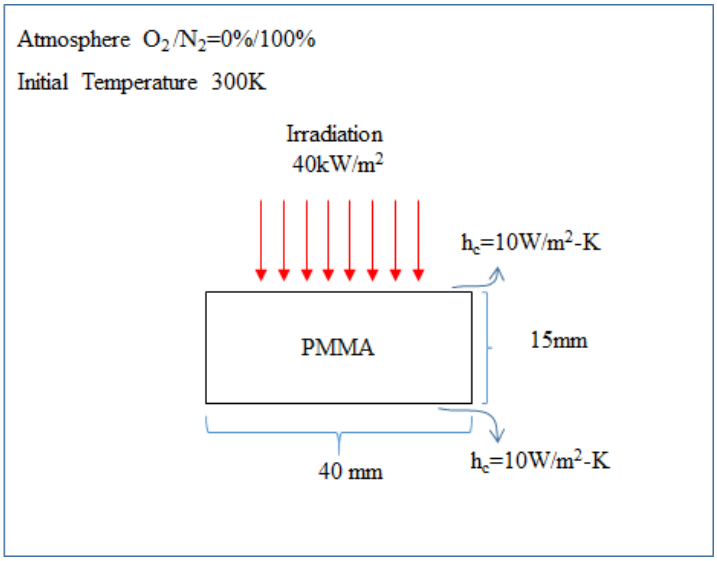

Figure 4-1 Schematic of gasification of PMMA

We assume the pyrolysis process consists of two reactions, where two condensed phase species and one gas phase species is taken into consideration. (Bpmma denotes for the “bubbled PMMA”. It has a larger porosity than the virgin pmma and thus allows gases to diffuse from the ambient.)

$$\text{pmma (s)} \rightarrow \text{bpmma (s)} \tag{4-1}$$

$$\text{bpmma (s)} \rightarrow \nu_{gas,product}\,\text{thermal pyrolysate (g)} \tag{4-2}$$

All of reaction rates are assumed to have a form shown as follow:

$$\dot{\omega}_k''' = Z_k e^{-E_k/RT}\left(\frac{\bar{\rho}Y_k\Delta z}{\left(\bar{\rho}Y_k\Delta z\right)_\Sigma}\right)^{n_i}\frac{\left(\bar{\rho}Y_k\Delta z\right)_\Sigma}{\Delta z}\left[\left(1+y_{O_2}\right)^{n_k}-1\right] \tag{4-3}$$

This is the reaction rate used in Gpyro. Note that this reaction rate is a volumetric term, for which the unit is kg/(m^3·s). It is different from the commonly seen normal reaction rate, for which the unit is 1/s.

The kinetic parameters and condensed phase properties required in solving this problem are listed in Table 4-1 and Table 4-2.

Table 4-1 Kinetic parameters for 1D pyrolysis problem [6]

Reaction No.	**Z** (s^{-1})	**E** (kJ/mol)	**ΔH_s** (J/kg)	**ΔH_v** (J/kg)	**n** (-)	**n_{O2}** (-)	**g^*_{O2}**	**$g^*_{gas,prod}$**
(4-1)	2.31E+10	115.3	0.00E+00	0.00E+00	1.04	0	0	0
(4-2)	4.89E+13	197.6	0.00E+00	7.28E+05	1.16	0	0	1

Table 4-2 Condensed phase properties for 1D pyrolysis problem [6]

Name	k_{0z} (W/m-K)	n_{kz} (-)	ρ_0 (kg/m^3)	n_r (-)	C_0 (J/kg-K)	n_c (-)	ε (-)	k (m^{-1})	γ (m)	K (m^2)	ρ_{s0} (m^3)
pmma	0.200	-0.190	1190	-0.12	1606.0	0.890	0.860	1.98E+03	0	10^{-10}	1200
bpmma	0.180	-0.180	1036	-0.14	1667.0	0.720	0.870	1.00E+03	0	10^{-10}	1200

4.2 Gpyro setting

4.2.1 General worksheet

DT0	0.1	Initial timestep (s)
TAMB	300	Ambient temperature, T_∞ (K)
TREF	300	Reference temperature, T_r (K)
P0	1.013E+05	Background pressure, P_0 (Pa)
GX	0.00	x-component of gravity vector (m/s^2)
GZ	0.00	z-component of gravity vector (m/s^2)
GY	0.00	y-component of gravity vector (m/s^2)
THERMAL_EQUILIBRIUM	.TRUE.	Assume thermal equilibrium between gas and solid phase?
VHLC	0.0	Volumetric heat loss coefficient (W/m^3-K)
HCV	1.00E+06	Volumetric heat transfer coefficient for solid-gas heat transfer, h_{cv} (W/m^3-K)
NU_A	2.00	Nu = a + b Re^c = h_{cv} d_p^2 / k_g
NU_B	1.00	Nu = a + b Re^c = h_{cv} d_p^2 / k_g
NU_C	0.50	Nu = a + b Re^c = h_{cv} d_p^2 / k_g
NTDMA_ITERATIONS	100	Number of times to iterate over all conservation eqns before reducing Δt
NSSPECIESITERNS	10	Number of local iterations for solid species eqn
NCONTINUITYITERNS	1	Number of local iterations for continuity eqn
ALPHA	-1	Global relaxation parameter, α
ALPHA_YIS	0.5	
ALPHA_YJG	0.2	
ALPHA_HG	1	
ALPHA_P	1	
ALPHA_H	1	
TMPTOL	1.00E-03	Temperature convergence criterion (absolute) in K
HTOL	1.00E-07	Convergence criterion for Newton extraction of T from weighted h (absolute, J/kg)
YITOL	1.00E-11	Relative tolerance (convergence criterion) for condensed-phase mass fractions
PTOL	1.00E-03	Absolute tolerance for convergence on pressure (Pa)
YJTOL	1.00E-04	Tolerance (relative) for convergence on gaseous species mass fractions
HGTOL	1.00E-01	Tolerance (absolute) for convergence on gaseous enthalpy (J/kg)
EXPLICIT_T	.FALSE.	Use T from previous timestep to evaluate rxn rates & thermal props?
SOLVE_GAS_YJ	.TRUE.	Solve conservation equations for individual gas species?
SOLVE_GAS_ENERGY	.FALSE.	Solve gas-phase energy equation?
SOLVE_PRESSURE	.TRUE.	Use Darcy's law to solve for pressure distribution?
USE_TOFH_NEWTON	.TRUE.	Use Newton iteration to get T from weighted h?
SHYI_CORRECTION	.TRUE.	Include "source" term for d/dz[(k/c)*h_i*dY_i/dz] ?
NCOEFF_UPDATE_SKIP	1	Eqn coefficients get updated every NCOEFF_UPDATE_SKIP iterations
FDSMODE	.FALSE.	Emulate FDS pyrolysis model and dump fds input file?
CONVENTIONAL_RXN_ORDER	.FALSE.	Use traditional treatment of reaction order?
NOCONSUMPTION	.FALSE.	Prevent cell thickness from changing due to material consumption by pyrolysis?
EPS	1.00E-10	When cell thickness decreases to this size (m) no further reactions occur
BLOWING	.FALSE.	Use Couette flow approximation to account for effect of blowing?
CONSTANT_DHVOL	.TRUE.	Use constant value of ΔH_{vol}?
FULL_QSG	.FALSE.	If THERMAL_EQUILIBRIUM = .TRUE., use complete expression for Q_{s-g}?
GASES_PRODUCED_AT_TSOLID	.FALSE.	If THERMAL_EQUILIBRIUM = .FALSE., are gases produced at solid temperature?
TORTUOSITY_FACTOR	1	
USE_TORTUOSITY_FACTOR_FOR_FLUX	.TRUE.	

Figure 4-2 The setting of General worksheet for 1D pyrolysis problem

General worksheet is where all the overall computational and physical parameters should be specified. The setting of it for this 1D problem is shown in Figure 4-2.

Two specific settings deserve our attention. First, to solve this problem, we might need to turn on the mode of separate relaxation parameter setting by setting ALPHA (global relaxation factor) to -1 (See 1.1), since IALPHA_YIS, ALPHA_YJG might need to be specified to 0.5 and 0.2 (You can get other values that might work as well) respectively to make this specific calculation converge.

As demonstrated in Section 1.1, an entry for setting tortuosity factor is added in V0.8175. Note that the default value for tortuosity is 0.1. However, in this case, no tortuosity needs to be considered. Thus, the tortuosity needs to be set back to 1.

4.2.2 SPROPS worksheet (Condensed phase species properties)

For solving this 1D problem, the setting in SPROPS worksheet is even easier than some TGA

problem, since all of parameters needed in the simulation has been given in . What we have to do is to copy all of these parameters into SPROPS worksheet as shown in Figure 4-3.

However, it should be noted that in real computational study the determination of the properties of condensed phase species is one of the hardest parts in our research, since it is not practical and economically prohibitive for us to measure all of the physical properties every time we conduct a specific case study.

In this problem, all of these parameters (listed in Table 4-1 and Table 4-2) are obtained through inverse modelling[6]. More details about inverse modelling can be found in [7].

2	NSPEC	# of condensed-phase species														
Enter properties for individual condensed-phase species below:																
ISPEC	Name	k_{0z} (W/m-K)	n_{kz} (-)	ρ_0 (kg/m^3)	n_p (-)	c_0 (J/kg-K)	n_c (-)	ε (-)	κ (m^{-1})	T_m (K)	ΔH_m (J/kg)	σ^2_m (K^2)	γ (m)	K_z (m^2)	ρ_{s0} (kg/m^3)	d_p (m)
1	pmma	0.200	-0.190	1190	-0.12	1606.0	0.890	0.860	1.98E+03	3000	0.00E+00	0	0.00E+00	1D-10	1200.0	5.00E-04
2	bpmma	0.180	-0.180	1036	-0.14	1667.0	0.720	0.870	1.00E+03	3000	0.00E+00	0	0.00E+00	1D-10	1200.0	5.00E-04

Figure 4-3 The setting of SPROPS worksheet for 1D pyrolysis problem

4.2.3 RXNS worksheet (Condensed phase reactions)

Likewise, for the setting of RXNS worksheet all we need to do is to copy the parameters listed in Table 4-1 into the worksheet. One thing should be pointed out is that, for the first reaction, χ should be set to 0. **The physical meaning of this setting is that there is no gas produced in the reaction, but the condensed phase species would undergoes intumescence, as the density of bpmma is smaller than pmma.**

2	nrxns	# of reactions														
Specify reactions below. If 'To' species is not the name of a species specified in the 'props' worksheet, it is assumed to be gaseous																
IRXN	From (species A)	To (species B)	Z (s^{-1})	E (kJ/mol)	ΔH_s (J/kg)	ΔH_v (J/kg)	χ (-)	n (-)	n_{O2} (-)	$i_{kinetic\ model}$	$i_{O2\ rxn}$	m (-)	K_{cat} (-)	i_{cat}	T_{crit} (K)	
1	pmma	bpmma	2.31E+10	115.3	0.00E+00	0.00E+00	0	1.04	0	0	0	0	0	0	0	
2	bpmma	gases	4.89E+13	197.6	0.00E+00	7.28E+05	1	1.16	0	0	0	0	0	0	0	

Figure 4-4 The setting of RXNS Worksheet for 1D pyrolysis problem

4.2.4 GpyroS worksheet (Gas phase species properties)

Different from 0D simulation, gas properties cannot be set to arbitrary values now, since they are very important part in the calculation of 1D problem. In this specific case, three types of gas species should be specified as shown in Figure 4-5. σ, ε/k are Lenard-Jones parameters, which are used for calculating mass diffusivity of gas species. For the commonly seen gas species, their Lenard Jones parameters can be found in [8]. Note that the gas product is assumed to have the same thermal dynamic properties of CO_2.

3	NGSPEC	# of gaseous species
1	IBG	Species index of background gaseous species (for calculating diffusivity)
2	IO2	Species index of oxygen
1100	CPG	Specific heat capacity of gas (J/kg-K)

IGSPEC	Name	M (g/mol)	σ (Å)	ε/k (K)	c_{p0} (J/kg-K)	n_c (-)
1	thermal_pyrolysate	44	3.996	190	1100	0.00
2	oxygen	32	3.434	113	1100	0.00
3	nitrogen	28	3.667	99.8	1100	0.00

Figure 4-5 The setting of GPROPS worksheet for 1D pyrolysis problem

4.2.5 GYIELDS worksheet (Gas yields matrix)

The setting in GYILEDS worksheet is simple as shown below. Note that even though first reaction has no gas product, we still have to make sure the sum of gas yields is 1 rather than 0. Although this setting has no physical meaning, it is necessary to make the input file successfully read by Gpyro solver.

3	NGSPEC	# of gaseous species	
		Reaction number ->	
		1	2
	From	pmma	bpmma
	To	bpmma	gases
	Z	2.31E+10	4.89E+13
	E	115.3	197.6
	ΔH_s	0.00E+00	0.00E+00
	ΔH_v	0.00E+00	7.28E+05
	χ	0.00	1.00
	n	1.04	1.16
	n_{O2}	0.00	0.00
		Yields matrix:	
		Reaction number ->	
IGSPEC	Name	1	2
1	thermal_pyrolysate	0	1.00
2	oxygen	0.00	0.00
3	nitrogen	1.00	0.00
4	0	0	0.00
5	0	0	0.00
6	0	0.00	0.00
7	0	0.00	0.00
8	0	0.00	0.00
9	0	0.00	0.00
10	0	0.00	0.00
	TOTALS:	1.00	1.00

Figure 4-6 The setting of GYIELDS worksheet for 1D pyrolysis problem

4.2.6 IC worksheet (Initial conditions)

The initial condition is specified as below:

1	NIC	Number of initial conditions groups to apply						
Enter layer information below:								
IC #	T_0 (K)	T_{g0} (K)	P_0 (Pa)	$Y_{i0,1}$ (-)	$Y_{i0,2}$ (-)	$Y_{j0,1}$ (-)	$Y_{j0,2}$ (-)	$Y_{j0,3}$ (-)
1	300.0	300.0	101300.0	1.000	0.000	0.000	0.000	1.000

Figure 4-7 The setting of IC worksheet for 1D pyrolysis problem

4.2.7 GEOM and BC worksheet (Geometry and boundary conditions)

In GEOM worksheet, the dimension of sample and grid spacing should be specified. Here the grid spacing is chosen to be 0.01mm and the number of cell is therefore specified to 151 (=1.5/0.01+1). For top surface (DEFAULT_SURF_IDX(5)) and bottom surface(DEFAULT_SURF_IDX(6)), two boundary conditions are specified in BC worksheet and transferred by the boundary condition index string-SURF_IDF.

1	NMESH	Number of gpyro meshes		
0	NOBST	Number of OBST's		
	Mesh 01	Mesh 02	Mesh 03	
ZDIM	0.015			
NCELLZ	151			
XDIM	0.04			
NCELLX	1			
YDIM	1			
NCELLY	1			
GEOMETRY_FILE	'null'			
DEFAULT_SURF_IDX(1)	0			
DEFAULT_SURF_IDX(2)	0			
DEFAULT_SURF_IDX(3)	0			
DEFAULT_SURF_IDX(4)	0			
DEFAULT_SURF_IDX(5)	1			
DEFAULT_SURF_IDX(6)	2			
DEFAULT_IC	1			
OFFSETZ	0			
OFFSETX	0			
OFFSETY	0			

Figure 4-8 The setting of GEOM worksheet for 1D pyrolysis problem

The setting for boundary conditions is very important in the simulation study, especially in Gpyro, since no error report will be given if a wrong boundary condition is set in BC worksheet. This worksheet should be cautiously specified.

In this case, all of the boundary conditions for top surface are specified in the first line, while that for bottom surface are set in the second line.

		Solid Energy						Gas momentum	
SURF_IDX	t (s)	q_e (W/m^2)	h_c (W/m^2-K)	~~η_{bc}~~ (-)	T_∞ (K)	Reradiation?	Fixed T (K)	m" (g/m^2-s)	P (Pa)
1		40000	10	~~0~~	300	.TRUE.	-1	0	101300
2		0	10	~~0~~	300	.FALSE.	-1	0	-1000

(a)

Gas energy				Gas species					
q_e (W/m^2)	h_c (W/m^2-K)	T_∞ (K)	Fixed T (K)	h_m (kg/m^2-s)	Y_{j1} (-)	Y_{j2} (-)	Y_{j3} (-)	Y_{j4} (-)	Y_{j5} (-)
0	12	300	-1000	0.00909091	0.000	0.000	1.000	0.000	0
0	12	300	-1000	0	0.000	0.000	1.000	0.000	0

(b)

Figure 4-9 The setting of GEOM worksheet for 1D pyrolysis problem

1. **Condensed phase energy boundary conditions**

The top face boundary condition can be expressed as below

$$-\bar{k}\left.\frac{\partial T}{\partial z}\right|_{z=0} = -h_c\left(T\big|_{z=0} - T_\infty\right) - \bar{\varepsilon}\sigma\left(T^4\big|_{z=0} - T_\infty^4\right) \tag{4-4}$$

h_c, T_∞ is specified in The "Solid energy" section, setting 'TURE' in the entry of 'Reradiation?' means to include the radiation term $\bar{\varepsilon}\sigma\left(T^4\big|_{z=0} - T_\infty^4\right)$ in calculation.

The back face boundary condition is:

$$-\bar{k}\left.\frac{\partial T}{\partial z}\right|_{z=\delta} = h_{c\delta}\left(T\big|_{z=\delta} - T_\infty\right) \tag{4-5}$$

Since only convective heat transfer is considered for bottom face, so only h_c needs to be specified.

2. **Gas momentum boundary conditions**

The boundary condition at the front face sets the pressure equal to the atmospheric value:

$$P\big|_{z=0} = P_\infty \tag{4-6}$$

The pressure gradient at the back face is set to zero to give an impermeable back face:

$$\left.\frac{\partial P}{\partial z}\right|_{z=\delta} = 0 \tag{4-7}$$

A boundary condition like this can be specified by setting a negative value for pressure with no gaseous mass flux.

3. Gas species boundary conditions

In this problem, boundary condition at top face is expressed as follow

$$-\bar{\psi}\rho_g D\left.\frac{\partial Y_j}{\partial z}\right|_{z=0} \approx h_m\left(Y_j^{\infty} - Y_j\big|_{z=0}\right) \tag{4-8}$$

Where the diffusive coefficient, h_{m}, is obtained using mass/heat transport analogy, i.e assuming

$$h_m \approx \frac{h_c}{c_{pg}} \tag{4-9}$$

Therefore, in this case h_{m} is set to $\frac{h_c}{c_{pg}} = \frac{10}{1100}$.

At bottom face, gaseous mass fraction gradient is set to zero to give an impermeable boundary condition

$$\left.\frac{\partial Y_j}{\partial z}\right|_{z=\delta} = 0 \tag{4-10}$$

Which can be specified by setting h_m to 0.

Since gas energy equations are not solved in this problem, so the boundary condition in this part can be set arbitrarily.

4.2.8 CASES worksheet (Batch mode setting)

The setting in CASES worksheet is simple as below:

1	Number of cases to run			
Case #	IMESH	t_{stop} [s]	0D?	β [K/min]
1	1	180	.FALSE.	0.0

Figure 4-10 The setting of CASES worksheet for 1D pyrolysis problem

4.3 Simulation results

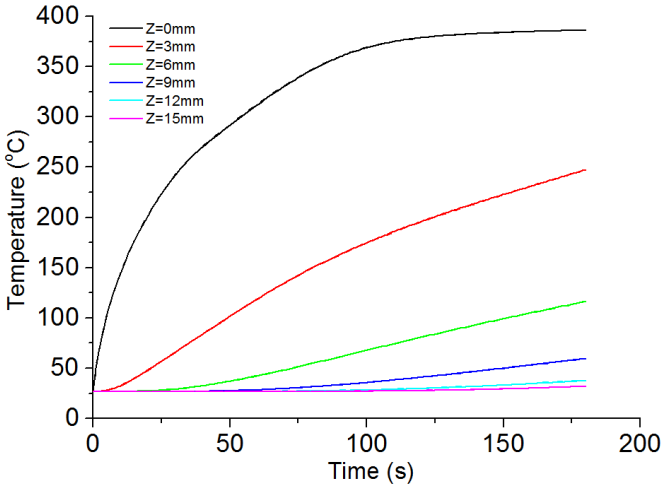

Figure 4-11 Temperature profile

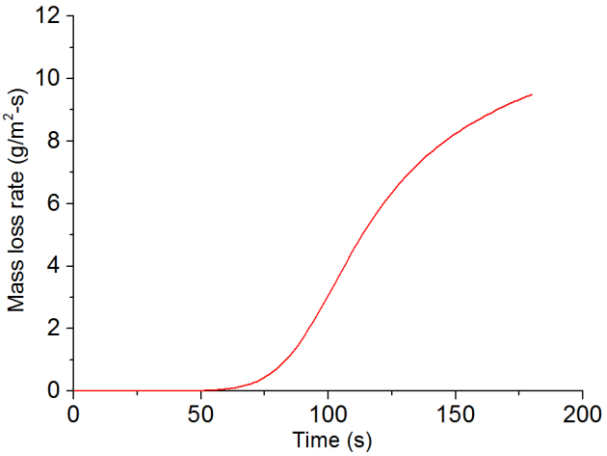

Figure 4-12 Mass loss rate as a function of temperature

The simulation solution to the 1D smouldering problem is displayed above. The results also match well with the original work[6].

5 Problem IV: 1D smouldering

In 1996, NASA conducted a smouldering experiment on space station to investigate how smoulder wave propagates in polyurethane foam (12cm in diameter and 14 cm length) under mirco-gravity environment. Lautenberger and Fernandez-Pello [6] have simulated this experiment in their paper. Here this paper is adapted to a 1D smouldering problem.

5.1 Problem Statement

Figure 5-1 is the shematic of this problem. A sample of polyurethane foam is ignited by an igniter placed at the bottom face. Air is forced to flow through the sample from the bottom to the top. Air flow velocity remains at 0.1mm/s during the first 400s. Afterwards, the velocity is increased to 5mm/s. The convective heat losses is considered on both top and side faces. For the top face, the heat transfer coefficient is assumed to be 10W/m^2-K. The heat losses on side faces is taken into account by adding a volumetric heat loss term in the condensed-phase energy equation, the heat loss coefficient is assumed to be 25W/m^2-K. The experimental temperature curve is applied as the boundary condition at bottom face.

Can you use Gpyro to simulate this problem and predict how temperature at different depths evolve with time?

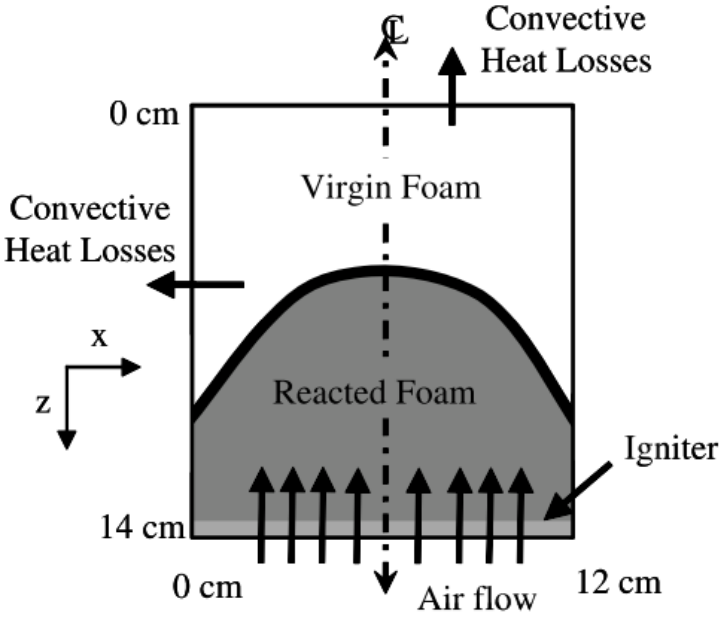

Figure 5-1 Schematic of mirco-gravity Smouldering of polyurethane foam [9].

This smouldering process is assumed to have a kinetic scheme developed by Dodd, Lautenberger

[9]. Seven reactions are included in this scheme and five condensed phase species are tracked.

$$\text{foam (s)} \rightarrow \nu_{\beta,1}\text{beta\_foam (s)} + \nu_{p,1}\text{thermal\_pyrolysate (g)} \tag{5-1}$$

$$\text{beta\_foam (s)} \rightarrow \nu_{tc,2}\text{thermal\_char (s)} + \nu_{p,2}\text{thermal\_pyrolysate (g)} \tag{5-2}$$

$$\text{thermal\_char (s)} \rightarrow \text{thermal\_pyrolysate (g)} \tag{5-3}$$

$$\text{foam (s)} + \nu_{o,4}\text{O}_2 \rightarrow \nu_{c,4}\text{char (s)} + \nu_{p,4}\text{oxidative\_pyrolysate (g)} \tag{5-4}$$

$$\text{beta\_foam (s)} + \nu_{o,5}\text{O}_2 \rightarrow \nu_{c,5}\text{char (s)} + \nu_{p,5}\text{oxidative\_pyrolysate (g)} \tag{5-5}$$

$$\text{char (s)} + \nu_{o,6}\text{O}_2 \rightarrow \nu_{\alpha,6}\text{alpha\_char (s)} + \nu_{p,6}\text{oxidative\_pyrolysate (g)} \tag{5-6}$$

$$\text{alpha\_char (s)} \rightarrow \text{products (s)} \tag{5-7}$$

All of reaction rates are assumed to have a form shown as (4-3).

The kinetic parameters and condensed phase properties required in solving this problem are listed in Table 5-1 and Table 5-2.

Table 5-1 Kinetic parameters for 1D smouldering problem [6]

Reaction No.	**Z**	**E**	**ΔH_s**	**ΔH_v**	**n**	**n_{O2}**	**g^*_{O2}**	**$g^*_{gas,prod}$**
	(s^{-1})	**(kJ/mol)**	**(J/kg)**	**(J/kg)**	**(-)**	**(-)**		
(5-1)	3.16E+18	227	4.00E+04	4.00E+04	0.80	0	0	1
(5-2)	1.29E+10	146.5	7.50E+05	7.50E+05	1.25	0	0	1
(5-3)	8.24E+08	173.3	2.50E+06	2.50E+06	0.92	0	0	1
(5-4)	1.37E+15	188	1.50E+06	1.50E+06	0.48	1	-0.3	1.3
(5-5)	1E+16	200	1.60E+06	1.60E+06	0.52	1	-0.4	1.4
(5-6)	1E+15	201	2.50E+06	2.50E+06	1.30	1	-1.5	2.5
(5-7)	4.25E+08	153	2.50E+06	2.50E+06	1.61	1	-1.5	2.5

* g denotes gas yield factor[2]

Table 5-2 Condensed phase properties for 1D smouldering problem [6]

Name	**k_{0z}**	**n_{kz}**	**ρ_0**	**n_r**	**C_0**	**n_c**	**ε**	**k**	**γ**	**K**	**ρ_{s0}**
	(W/m-K)	**(-)**	**(kg/m^3)**	**(-)**	**(J/kg-K)**	**(-)**	**(-)**	**(m^{-1})**	**(m)**	**(m^2)**	**(m^3)**

foam	0.050	1.600	26.5	0	1760.0	0.700	1.00	1.00E+07	0.001	5.20E-09	900
βfoam	0.050	1.600	18	0	1760.0	0.700	1.00	1.00E+07	0.001	1.00E-08	900
Tchar*	0.050	1.600	1.1	0	1760.0	0.700	1.00	1.00E+07	0.001	3.00E-08	900
char	0.050	1.600	10	0	1760.0	0.700	1.00	1.00E+07	0.001	3.00E-08	900
αchar	0.050	1.600	2.4	0	1760.0	0.700	1.00	1.00E+07	0.001	3.00E-08	900

* Tchar represents thermal_char

5.2 Gpyro setting

5.2.1 General worksheet

DT0	0.1	Initial timestep (s)
TAMB	300	Ambient temperature, T_∞ (K)
TREF	300	Reference temperature, T_r (K)
P0	1.013E+05	Background pressure, P_0 (Pa)
GX	0.00	x-component of gravity vector (m/s^2)
GZ	0.00	z-component of gravity vector (m/s^2)
GY	0.00	y-component of gravity vector (m/s^2)
THERMAL_EQUILIBRIUM	.TRUE.	Assume thermal equilibrium between gas and solid phase?
VHLC	25.0	Volumetric heat loss coefficient (W/m^3-K)
HCV	1.00E+06	Volumetric heat transfer coefficient for solid-gas heat transfer, h_{cv} (W/m^3-K)
NU_A	2.00	Nu = a + b Re^c = h_{cv} d_p^2 / k_g
NU_B	1.00	Nu = a + b Re^c = h_{cv} d_p^2 / k_g
NU_C	0.50	Nu = a + b Re^c = h_{cv} d_p^2 / k_g
NTDMA_ITERATIONS	100	Number of times to iterate over all conservation eqns before reducing Δt
NSSPECIESITERNS	1	Number of local iterations for solid species eqn
NCONTINUITYITERNS	1	Number of local iterations for continuity eqn
ALPHA	1	Global relaxation parameter, α
ALPHA_YIS	0.5	
ALPHA_YJG	0.2	
ALPHA_HG	1	
ALPHA_P	1	
ALPHA_H	1	
TMPTOL	1.00E-03	Temperature convergence criterion (absolute) in K
HTOL	1.00E-07	Convergence criterion for Newton extraction of T from weighted h (absolute, J/
YITOL	1.00E-04	Relative tolerance (convergence criterion) for condensed-phase mass fraction
PTOL	1.00E-03	Absolute tolerance for convergence on pressure (Pa)
YJTOL	1.00E-04	Tolerance (relative) for convergence on gaseous species mass fractions
HGTOL	1.00E-01	Tolerance (absolute) for convergence on gaseous enthalpy (J/kg)
EXPLICIT_T	.FALSE.	Use T from previous timestep to evaluate rxn rates & thermal props?
SOLVE_GAS_YJ	.TRUE.	Solve conservation equations for individual gas species?
SOLVE_GAS_ENERGY	.FALSE.	Solve gas-phase energy equation?
SOLVE_PRESSURE	.TRUE.	Use Darcy's law to solve for pressure distribution?
USE_TOFH_NEWTON	.TRUE.	Use Newton iteration to get T from weighted h?
SHYI_CORRECTION	.TRUE.	Include "source" term for d/dz[(k/c)*h_i*dY$_i$/dz] ?
NCOEFF_UPDATE_SKIP	1	Eqn coefficients get updated every NCOEFF_UPDATE_SKIP iterations
FDSMODE	.FALSE.	Emulate FDS pyrolysis model and dump fds input file?
CONVENTIONAL_RXN_ORDER	.FALSE.	Use traditional treatment of reaction order?
NOCONSUMPTION	.FALSE.	Prevent cell thickness from changing due to material consumption by pyrolysis
EPS	1.00E-10	When cell thickness decreases to this size (m) no further reactions occur
BLOWING	.FALSE.	Use Couette flow approximation to account for effect of blowing?
CONSTANT_DHVOL	.TRUE.	Use constant value of ΔH_{vol}?
FULL_QSG	.FALSE.	If THERMAL_EQUILIBRIUM = .TRUE., use complete expression for Q_{s-g}?
GASES_PRODUCED_AT_TSOLID	.FALSE.	If THERMAL_EQUILIBRIUM = .FALSE., are gases produced at solid temperatu
TORTUOSITY_FACTOR	1	

Figure 5-2 The setting of GENERAL worksheet for 1D smouldering problem

The setting for GENERAL worksheet is shown by Figure 5-2. Most of them can be kept the same as default, except for two parameters: VHLC and TORTUOSITY_FACTOR. VHLC is volumetric heat

loss coefficient, which can be applied to account for the convective heat losses on the faces that cat not to modeled in 1D simulation. In this specific case, these faces are two side faces and VHLC should be set to 25W/m^2-K.

As what is described in 4.2.1, TORTUOSITY_FACTOR needs to be set back to 1.

5.2.2 SPROPS worksheet (Condensed phase species properties)

No particular setting is worth noting in SPROPS worksheet. What we need to do is to copy all of parameters listed in Table 5-2 into the worksheet as shown in Figure 5-3

5	NSPEC	# of condensed-phase species													
Enter properties for individual condensed-phase species below:															
ISPEC	Name	k_{0z} (W/m-K)	n_{kz} (-)	ρ_0 (kg/m^3)	n_ρ (-)	c_0 (J/kg-K)	n_c (-)	ε (-)	κ (m^{-1})	T_m (K)	ΔH_m (J/kg)	σ^2_m (K^2)	γ (m)	K_z (m^2)	ρ_{s0} (kg/m^3)
1	foam	0.050	1.600	26.5	0	1760.0	0.700	1.000	1.00E+07	3000	0.00E+00	0	1.00E-03	5.20E-09	900.0
2	beta_foam	0.050	1.600	18	0	1760.0	0.700	1.000	1.00E+07	3000	0.00E+00	0	1.00E-03	1.00E-08	900.0
3	thermal_char	0.050	1.600	1.1	0	1760.0	0.700	1.000	1.00E+07	3000	0.00E+00	0	1.00E-03	3.00E-08	900.0
4	char	0.050	1.600	10	0	1760.0	0.700	1.000	1.00E+07	3000	0.00E+00	0	1.00E-03	3.00E-08	900.0
5	alpha_char	0.050	1.600	2.4	0	1760.0	0.700	1.000	1.00E+07	3000	0.00E+00	0	1.00E-03	3.00E-08	900.0

Figure 5-3 The setting of SPROPS worksheet for 1D smouldering problem

5.2.3 RXNS worksheet (Condensed phase reactions)

Likewise, for the setting of RXNS worksheet all we need to do is to copy the parameters listed in Table 5-1 into the worksheet.

7	nrxns	# of reactions													
Specify reactions below. If 'To' species is not the name of a species specified in the 'props' worksheet, it is assumed to be gaseous															
IRXN	From (species A)	To (species B)	Z (s^{-1})	E (kJ/mol)	ΔH_s (J/kg)	ΔH_v (J/kg)	χ (-)	n (-)	n_{O2} (-)	$i_{kinetic\ model}$	$i_{O2\ rxn}$	m (-)	K_{cat} (-)	i_{cat}	T_{crit} (K)
1	foam	beta_foam	3.16E+18	227	4.00E+04	4.00E+04	1	0.80	0	0	0	0	0	0	0
2	beta_foam	thermal_char	1.29E+10	146.5	7.50E+05	7.50E+05	1	1.25	0	0	0	0	0	0	0
3	thermal_char	gases	8.24E+08	173.3	-2.50E+06	-2.50E+06	1	0.92	0	0	0	0	0	0	0
4	foam	char	1.37E+15	188	-1.50E+06	-1.50E+06	1	0.48	1	0	0	0	0	0	0
5	beta_foam	char	1E+16	200	-1.60E+06	-1.60E+06	1	0.52	1	0	0	0	0	0	0
6	char	alpha_char	1E+15	201	-2.50E+06	-2.50E+06	1	1.30	1	0	0	0	0	0	0
7	alpha_char	gases	4.25E+08	153	-2.50E+06	-2.50E+06	1	1.61	1	0	0	0	0	0	0

Figure 5-4 The setting of RXNS worksheet for 1D smouldering problem

5.2.4 GpyroS worksheet (Gas phase species properties)

In this case, five types of gas species should be specified as shown inFigure 5-5. σ and ε/k are Lenard-Jones parameters, which are used for calculating mass diffusivity of gas species. For the commonly seen gas species, their Lenard Jones parameters can be found in [8]. Note that the gas product is assumed to have the same thermodynamic properties of CO_2.

5	NGSPEC	# of gaseous species
1	IBG	Species index of background gaseous species (for calculating diffusivity)
2	IO2	Species index of oxygen
1100	CPG	Specific heat capacity of gas (J/kg-K)

IGSPEC	Name	M (g/mol)	σ (Å)	ε/k (K)	~~c_{p0} (J/kg-K)~~	~~n_c (-)~~
1	thermal_pyrolysate	44	3.996	190	~~1100~~	~~0.00~~
2	oxygen	32	3.434	113	~~1100~~	~~0.00~~
3	nitrogen	28	3.667	99.8	~~1100~~	~~0.00~~
4	oxidative_pyrolysate	44	3.996	190	~~1100~~	~~0.00~~
5	product	44	3.996	190	~~1100~~	~~0.00~~

Figure 5-5 The setting of GPROPS worksheet for 1D smouldering problem

5.2.5 GYIELDS worksheet (Gas yields matrix)

The setting of GYILEDS worksheet is simple as shown in Figure 5-6. Gas yield factors come from Table 5-1.

IGSPEC	Name	1	2	3	4	5	6	7
1	thermal_pyrolysate	1	1.00	1.00	0.00	0.00	0.00	0.00
2	oxygen	0.00	0.00	0.00	-0.30	-0.40	-1.50	-1.50
3	nitrogen	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	oxidative_pyrolysate	0	0.00	0.00	1.30	1.40	2.50	0.00
5	product	0	0.00	0.00	0.00	0.00	0.00	2.50
6	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	TOTALS:	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Figure 5-6 The setting of GYIELDS worksheet for 1D smouldering problem

5.2.6 IC worksheet (Initial conditions)

The initial condition is specified as below:

IC #	T_0 (K)	T_{g0} (K)	P_0 (Pa)	$Y_{i0,1}$ (-)	$Y_{i0,2}$ (-)	$Y_{i0,3}$ (-)	$Y_{i0,4}$ (-)	$Y_{i0,5}$ (-)	$Y_{j0,1}$ (-)	$Y_{j0,2}$ (-)	$Y_{j0,3}$ (-)	$Y_{j0,4}$ (-)	$Y_{j0,5}$ (-)
1	300.0	300.0	101300.0	1.000	0.000	0.0	0.0	0.0	0.000	0.230	0.770	0.000	0.000

Figure 5-7 The setting of IC worksheet for 1D smouldering problem

5.2.7 GEOM and BC worksheet (Geometry and boundary conditions)

In GEOM worksheet, shown in Figure 5-8, the dimension of sample and grid spacing should be specified. Here the grid spacing is chosen to be 0.01mm and the number of cell is therefore specified to 1400(14/0.01+1). For top surface (DEFAULT_SURF_IDX(5)) and bottom surface (DEFAULT_SURF_IDX(6)), two sets of boundary conditions are specified in BC worksheet and transferred via index string-SURF_IDF to GEOM worksheet.

1	NMESH	Number of gpyro meshes		
0	NOBST	Number of OBST's		
	Mesh 01	Mesh 02	Mesh 03	
ZDIM	0.14			
NCELLZ	1401			
XDIM	0.12			
NCELLX	1			
YDIM	1			
NCELLY	1			
GEOMETRY_FILE	'null'			
DEFAULT_SURF_IDX(1)	0			
DEFAULT_SURF_IDX(2)	0			
DEFAULT_SURF_IDX(3)	0			
DEFAULT_SURF_IDX(4)	0			
DEFAULT_SURF_IDX(5)	1			
DEFAULT_SURF_IDX(6)	2			
DEFAULT_IC	1			
OFFSETZ	0			
OFFSETX	0			
OFFSETY	0			

Figure 5-8 The setting of GEOM worksheet for 1D smouldering problem

The boundary condition is specified as shown in Figure 5-9. The boundary condition set for the bottom face is numbered as 2, while that for top face is 1. It should be noted that since a specified temperature curve (obtained from the experiment [10])is given as the boundary condition for the bottom face, we therefore have to split the curve into several segments and assume the linear increment within every segment (red marked).

		Solid Energy						Gas momentum	
SURF_IDX	t (s)	q_e (W/m^2)	h_c (W/m^2-K)	~~n_{hc} (-)~~	T_∞ (K)	Reradiation?	Fixed T (K)	m'' (g/m^2-s)	P (Pa)
1		0	10	0	300	.TRUE.	-1	0	101300
2	0	0	10	0	300	.FALSE.	300	0.1	-1000
2	400	0	10	0	300	.FALSE.	673	0.1	-1000
2	410	0	10	0	300	.FALSE.	685.5	5.8	-1000
2	440	0	10	0	300	.FALSE.	723	5.8	-1000
2	632	0	10	0	300	.FALSE.	783	5.8	-1000
2	780	0	10	0	300	.FALSE.	641	5.8	-1000
2	1000	0	10	0	300	.FALSE.	533	5.8	-1000
2	1200	0	10	0	300	.FALSE.	201	5.8	-1000

(a)

Gas species							
h_m (kg/m^2-s)	Y_{j1} (-)	Y_{j2} (-)	Y_{j3} (-)	Y_{j4} (-)	Y_{j5} (-)	Y_{j6} (-)	Y_{j6} (-)
0.0090901	0.000	0.230	0.770	0.000	0	0	0
0	0.000	0.230	0.770	0.000	0	0	0
0	0.000	0.230	0.770	0.000	0	0	0
0	0.000	0.230	0.770	0.000	0	0	0
0	0.000	0.230	0.770	0.000	0	0	0
0	0.000	0.230	0.770	0.000	0	0	0
0	0.000	0.230	0.770	0.000	0	0	0
0	0.000	0.230	0.770	0.000	0	0	0
0	0.000	0.230	0.770	0.000	0	0	0

(b)

Figure 5-9 The setting of BC worksheet for 1D smouldering problem

The meaning of boundary condition is explained as follow:

1. **Condensed phase energy boundary conditions**

The top face boundary condition can be expressed as below

$$-\bar{k}\left.\frac{\partial T}{\partial z}\right|_{z=0} = -h_c\left(T\big|_{z=0} - T_\infty\right) \tag{5-8}$$

h_c, T_∞ is specified in The "Solid energy" section.

The bottom face boundary condition is:

$$T_{z=\delta} = T_{\text{specifed}}(t) \tag{5-9}$$

2. **Gas momentum boundary conditions**

The boundary condition at the top face sets the pressure equal to the atmospheric value:

$$P\big|_{z=0} = P_\infty \tag{5-10}$$

The pressure gradient at the bottom face is set to zero to give an impermeable back face:

$$\left.\frac{\partial P}{\partial z}\right|_{z=\delta} = 0 \tag{5-11}$$

A boundary condition like this is specified by setting a negative value for pressure with no gaseous mass flux, as shown in Figure 5-9.

3. **Gas species boundary conditions**

In this problem, boundary condition at the top face is expressed as follow

$$-\bar{\psi}\rho_g D\left.\frac{\partial Y_j}{\partial z}\right|_{z=0} \approx h_m\left(Y_j^\infty - Y_j\big|_{z=0}\right) \tag{5-12}$$

Where the diffusive coefficient, h_{m}, is obtained using mass/heat transport analogy, i.e assuming

$$h_m \approx \frac{h_c}{c_{pg}} \tag{5-13}$$

Therefore, in this case h_{m} is set to $\frac{h_c}{c_{pg}} = \frac{10}{1100}$.

At the bottom face, gaseous mass fraction gradient is set to zero to give an impermeable boundary condition

$$\left.\frac{\partial Y_j}{\partial z}\right|_{z=\delta} = 0 \tag{5-14}$$

Which can be specified by setting h_m to 0.

Since gas energy equations are not solved in this problem, so the boundary condition in this part can be set arbitrarily.

5.2.8 CASES worksheet (Batch mode setting)

The setting in CASES worksheet is simple as below:

1	Number of cases to run			
Case #	IMESH	t_{stop} [s]	0D?	β [K/min]
1	1	1000	.FALSE.	0.0

Figure 5-10 The setting of CASES worksheet for 1D smouldering problem

5.3 Simulation results

The simulation solution to the 1D smouldering problem is displayed in Figure 5-11 and Figure 5-12. The results match well with the original work[6].

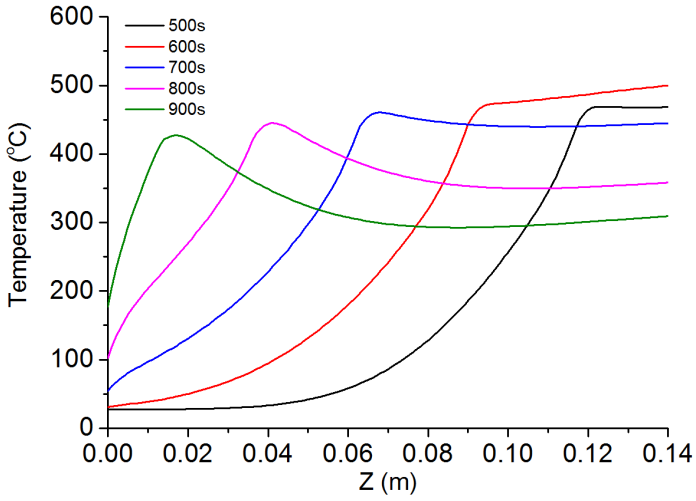

Figure 5-11 Temperature profile at different time

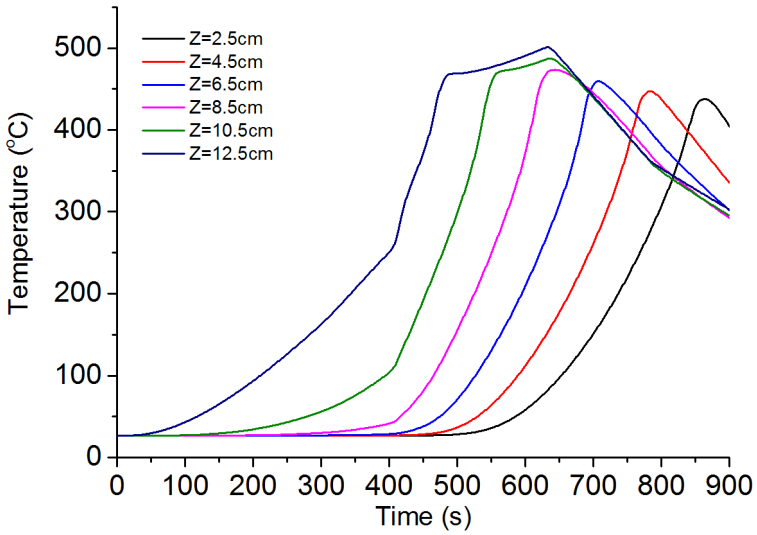

Figure 5-12 Temperature histories at different depths

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