Burn (BUR) Package
Users' Guide

The Burn (BUR) package models the combustion of gases in control volumes. The models consider the effects of burning on a global basis without modeling the actual reaction kinetics or tracking the actual flame front propagation. The BUR package models are based on the deflagration models in the HECTR 1.5 code. New in MELCOR 1.8.5 is a diffusion flame model, also derived from HECTR 1.5.

This Users' Guide describes the input to the BUR package, including a brief description of the models employed, the input format, sample input, discussion of the output, sensitivity coefficients, plot variables, and control variables. Details on the models can be found in the BUR Package Reference Manual.

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1. Introduction

The Burn (BUR) package models the combustion of gases in control volumes. The bulk burn models consider the effects of burning of premixed gases without modeling the actual reaction kinetics or tracking the actual flame front propagation. New in MELCOR 1.8.5 is a simple diffusion flame model which allows for the burning of hydrogen rich mixtures upon entry to volumes containing oxygen. The models in the BUR package are based on the models in the HECTR 1.5 code. The only significant modifications made were to provide more direct user control of the models through the implementation of sensitivity coefficients and to include optional model parameters that are used to override the nominal parameters in control volumes in which direct containment heating (DCH) is occurring. Note that the diffusion flame model can be used to model the burning occurring during DCH while leaving the bulk burn parameters at their nominal values.

Deflagrations are ignited if the mole fraction composition in a control volume satisfies a form of LeChatelier's formula. Tests for sufficient H_2 and O_2 are performed, as well as an inerting test for the presence of excessive diluents (H_2O and CO_2). Deflagrations are propagated into adjoining control volumes if additional tests for the H_2 and CO mole fractions in those volumes are satisfied and if the flow path is open to gas flow (i.e., the area is nonzero and the flow path is not covered by water). There is, however, no test for check valves.

The combustion rate is determined by the flame speed, the volume characteristic dimension, and the combustion completeness. The flame speed and combustion completeness can each be input as constant values, or they may be calculated from either user-specified control functions or the default HECTR correlations. The latter are derived from experimental data and depend on combustible and diluent gas concentrations.

For user convenience, the BUR package also prints messages to warn the user when the detonability criteria are satisfied in a control volume. However, only deflagrations are modeled; detonations are merely flagged.

Note: The gases hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), and oxygen (O_2) must be defined in the NonCondensible Gas (NCG) package whenever the BUR package is active. Steam (H_2O) is automatically present for all MELCOR calculations, so no special action need be taken to include it in a calculation.

2. User Input

The input for the BUR package consists of combustion parameters in the MELGEN and MELCOR input and timestep values for the start of each burn in the MELCOR input. If a BUR record is included in the user's input, all entries for that record must be included, except for cases noted in the following description:

2.1 MELGEN Input

BUR000 - Activation Record
Optional

This record activates the BUR package.

(1) IACTV - Activation Parameter
= 0, BUR package active
= 1, BUR package not active
(type = integer, default = 1, units = none)

BUR001 - Ignition Parameters
Optional

The ignition parameters for deflagrations are input on this record. Input for the first six or all ten entries must be specified if this record is included. See Section 2.2 of the Burn Package Reference Manual.

(1) XH2IGN - H_2 mole fraction limit for ignition without igniters.
(type = real, default = 0.10, units = none)

(2) XCOIGN - CO mole fraction limit for ignition without igniters.
(type = real, default = 0.167, units = none)

(3) XH2IGY - H_2 mole fraction limit for ignition with igniters.
(type = real, default = 0.07, units = none)

(4) XCOIGY - CO mole fraction limit for ignition with igniters.
(type = real, default = 0.129, units = none)

(5) XO2IG - Minimum O_2 mole fraction for ignition.
(type = real, default = 0.05, units = none)

(6) XMSCIG - Maximum H_2O plus CO_2 mole fraction for ignition.
(type = real, default = 0.55. units = none)

(7) XH2DCH - H_2 mole fraction limit for ignition during DCH.
(type = real, default = XH2IGY, units = none)

(8) XCODCH - CO mole fraction limit for ignition during DCH.
(type = real, default = XCOIGY, units = none)

(9) XO2DCH - O_2 mole fraction limit for ignition during DCH.
(type = real, default = XO2IG, units = none)

(10) XINDCH - H_2O plus CO_2 mole fraction limit for ignition during DCH.
(type = real, default = XMSCIG, units = none)

BUR002 - Detonation Parameters
Optional

The parameters to indicate a detonation are input on this record. Input for all three entries must be specified if this record is included. See Section 2.7 of the Burn Package Reference Manual.

(1) XH2DET - Minimum H_2 mole fraction for detonation.
(type = real, default = 0.14, units = none)

(2) XO2DET - Minimum O_2 mole fraction for detonation.
(type = real, default = 0.09, units = none)

(3) XH2ODT - Maximum H_2O mole fraction for detonation.
(type = real, default = 0.30, units = none)

BUR003 - Combustion Completeness and Propagation Parameters
Optional

The parameters controlling the extent of combustion and propagation to connected volumes are input on this record. Input for either the first eight or all ten entries must be specified if this record is included. See Sections 2.3 and 2.6 of the Burn Package Reference Manual.

(1) XH2CC - H_2 mole fraction value for calculating combustion completeness.
(type = real, default = 0.08, units = none)

(2) XCOCC - CO mole fraction value for calculating combustion completeness.
(type = real, default = 0.148, units = none)

(3) XH2PUP - H_2 mole fraction limit for upward propagation.
(type = real, default = 0.041, units = none)

(4) XCOPUP - CO mole fraction limit for upward propagation.
(type = real, default = 0.125, units = none)

(5) XH2PHO - H_2 mole fraction limit for horizontal propagation.
(type = real, default = 0.06, units = none)

(6) XCOPHO - CO mole fraction limit for horizontal propagation.
(type = real, default = 0.138, units = none)

(7) XH2PDN - H_2 mole fraction limit for downward propagation.
(type = real, default = 0.09, units = none)

(8) XCOPDN - CO mole fraction limit for downward propagation.
(type = real, default = 0.150, units = none)

(9) XH2CCD - Value of XH2CC during DCH.
(type = real, default = XH2CC, units = none)

(10) XCOCCD - Value of XCOCC during DCH.
(type = real, default = XCOCC, units = none)

BUR004 - Plot Edit Control
Optional

The plot edits requested by the BUR package are controlled by this input.

(1) IFLAGS - Plot controlling variable.
≥ 0, Plot edit will be requested at start and end of each burn if control function number IFLAGS is true; no BUR plot edits will be requested if it is false.
= -1, Plot edits will be requested at the start and end of each burn.
= -2, No plot edits will be requested by the BUR package.
(type = integer, default = -1, units = none)

BUR005 - Diffusion flame activation and burn parameters
Optional

This record activates the diffusion flame model and specifies the burn parameters for the flame. The default values are set to essentially burn most of the incoming hydrogen and CO in a flow path during DCH, and are quite different than the typical settings for the bulk burn model.

(1) IACTF - Diffusion flame model activation flag. Default is 0 (off); set to 1 (on) to activate model.
= 0, Off
= 1, On

(type = integer, default = 0, units = none)

(2) XH2FLM - Minimum hydrogen mole fraction of the flow path to burn. This should be set lower than the usual bulk burn default for realistic simulation (default is 0.0; and up to about 0.03 is reasonable).
(type = real, default = 0.0, units = none)

(3) XCOFLM - Minimum carbon monoxide mole fraction of the flow path to burn. Default is typical of bulk burn during DCH.
(type = real, default = 0.129, units = none)

(4) XO2FLM - Minimum oxygen mole fraction in downstream control volume to burn.
(type = real, default = 0.01, units = none)

(5) XSCFLM - Maximum inerting gas concentration in downstream control volume (steam+carbon dioxide) before burn stops.
(type = real, default = 0.9, units = none)

(6) XH2CCF - Hydrogen mole fraction to use in the LeChatelier formula for the combustion completeness of the diffusion flame. This is set to the DCH bulk burn value as default.
(type = real, default = 0.08, units = none)

(6) XCOCCF - Carbon monoxide mole fraction to use in the LeChatelier formula for the combustion completeness of the diffusion flame. This is set to the DCH bulk burn value as default.
(type = real, default = 0.148, units = none)

BURCFxx - Diffusion flame combustion completeness parameters.
$01 \leq xx \leq 99$
Optional

This record specifies the diffusion flame combustion completeness parameters for a flow path. A constant completeness (CC) factor may be specified, or alternatively, the HECTR correlation is available, although the validity of the HECTR correlation for a diffusion flame is unknown.

(1) IFLNUM - Flow path number. Putting -1 as the flow path will cause the value of CC to be used for all flow paths.
(type = integer, default = none, units = none)

(2) ICCFLG - Option to use for combustion completeness. For all options, the completeness must satisfy $0.0 \leq CC \leq 1.0$.

= -1, use constant CC.
= 0, use HECTR correlation.

(3) CC - Combustion completeness, $0.0 \le CC \le 1.0$.

BUR1XX - Burn Rate and Propagation Speed Parameters
$01 \le XX \le 99$
Optional

The parameters determining the burn rate and the speed of propagation are on this record series. If fewer than four entries are included on the record, default values will be used for the remaining entries. See Sections 2.4, 2.5, and 2.6 of the Burn Package Reference Manual.

(1) ICVNUM - User control volume number.
(type = integer, default = none, units = none)

(2) IGNTR - Igniter variable
< 0, IGNTR variable (0 or 1) given by REAL control function number ABS(IGNTR)
= 0, igniter not active in control volume
= 1, igniter is active in control volume
= 86, burning prohibited in control volume
(type = integer, default = 0, units = none)

(3) CDIM - Characteristic dimension of control volume.
If –1 is input, the radius of a sphere whose volume is the control volume total volume $\{3V/(4\pi)\}^{1/3}$ will be used.
(type = real, default = -1, units = m)

(4) TFRAC - Time fraction of burn before propagation is allowed. It must satisfy $0.0 \le TFRAC \le 1$.
(type = real, default = 0.0, units = none)

(5) CDDH - Value of CDIM during DCH.
(type = real, default = CDIM, units = m)

(6) TFDH - Value of TFRAC during DCH.
(type = real, default = TFRAC, units = none)

BURCCXX - Combustion Completeness Option
$01 \leq XX \leq 99$
Optional

The parameters determining the option used to calculate the combustion completeness for each volume are on this record series. The first two entries are required if this record is present.

(1) ICVNUM - User control volume number. If -1 is entered, then this combustion completeness specification will be used in all the volumes except those redefined on subsequent BURCCXX records.
(type = integer, default = none, units = none)

(2) ICCFLG - Option to use for combustion completeness. For all options, the combustion completeness must satisfy $0.0 \leq CC \leq 1.0$.
< 0, use constant value for completeness. Input the constant as entry 3 on this record
= 0, use correlation (sensitivity coefficient C2202)
> 0, calculate completeness from control function ICCFLG
(type = integer, default = 0, units = none)

(3) CC - If ICCFLG < 0, this is the combustion completeness to use. Otherwise, a value is required as a placeholder, but will not be used, see entries (4) and (5).
(type = real, default = none, units = none)

(4) ICCDCH - Value of ICCFLG, during DCH.
(type = integer, default = ICCFLG, units = none).

(5) CCDH - Value of CC during DCH.
(type = real, default = CC, units = none)

BURFSXX - Flame Speed Option
$01 \leq XX \leq 99$
Optional

The parameters determining the option used to calculate the flame speed for each volume are on this record series. The first two entries are required if this record is present.

(1) ICVNUM - User control volume number. If -1 is entered, then this flame speed specification will be used in all the volumes except those redefined on subsequent BURFSXX records.
(type = integer, default = none, units = none)

(2) IFSFLG - Option specifying how the flame speed is determined.
< 0, use constant value for flame speed. Input the constant as entry 3 on this record
= 0, use correlation (sensitivity coefficient C2200)
> 0, calculate flame speed from control function IFSFLG
(type = integer, default = 0, units = m/s)

(3) FS - If IFSFLG < 0, enter the flame speed to use. Otherwise, a value is required as a placeholder, but will not be used, see entries (4) and (5).
(type = real, default = none, units = none)

(4) IFSDCH - Value of IFSFLG during DCH.
(type = integer, default = IFSFLG, units = none)

(5) FSDH - Value of FS during DCH.
(type = real, default = FS, units = m/s)

2.2 MELCOR Input

Records BUR001, BUR003, BUR004, BUR1XX, BURCCXX, and BURFSXX may also be included in MELCOR input for any restart. In addition, the initial timestep size at burn initiation can be controlled through the following record.

BURTIM - Burn Timestep Information
Optional

The information controlling the system timestep at the initiation of a burn is given on this record. (BUR or other packages may further reduce the size of this initial timestep if necessary and may control the size of subsequent timesteps.)

(1) BURNDT - Burn timestep variable
< 0.0 The first system timestep during a burn will be ABS(BURNDT) x Total time of burn
= 0.0 First system timestep is 0.2 s
> 0.0 The first system timestep is BURNDT
(type = real, default = 0., units = s)

3. Sensitivity Coefficients

The *sensitivity coefficient* feature in MELCOR is a powerful feature that gives the user the ability to change selected parameters in the physics models that would otherwise require modification of the Fortran source code. The use of sensitivity coefficients is described in Section 7 of the MELCOR EXEC Users' Guide.

3.1 BUR Sensitivity Coefficients

C2200 - Flame Speed Parameters

The flame speed in meters per second is evaluated from the equation

$$V = Vbase * Cdil$$

where Vbase and Cdil are calculated by the following expressions depending on the value of Ymax, which is the value of y (described below), at the start of the burn and XD, which is the diluent concentration at the start of the burn.

If $0.0 \le Y\max \le Y1$,

$$Vbase = C1 * Y\max + C2$$

If $Y1 < Y\max \le Y2$,

$$Vbase = \left[C1 + (C2 - C3)/Y1\right] * Y\max + C3$$

If $Y2 < Y\max \le Y3$,

$$Vbase = \left[C1 + (C2 - C3)/Y1 + (C3 - C4)/Y2\right] * Y\max + C4$$

If $Y3 < Y\max \le Y4$,

$$Vbase = \left[C1 + (C2 - C3)/Y1 + (C3 - C4)/Y2 + (C4 - C5)/Y3\right] * Y\max + C5$$

If $Y4 < Y\max \le Y5$,

$$Vbse = [C1 + (C2 - C3)/Y1 + (C3 - C4)/Y2 + (C4 - C5)/Y3 + (C5 - C6)/Y4] * Y\max + C6$$

If $Y5 < Y\max \le 1$,

$$Vbase = [C1 + (C2 - C3)/Y1 + (C3 - C4)/Y2 + (C4 - C5)/Y3 + (C5 - C6)/Y4 + (C6 - C7)/Y5] * Y\max + C7$$

If $0.0 \le Y\max \le Y2$,

$$Cdil = \max\,[C11, C8 + C9 * XD + C10 * XD^2]$$

If $Y2 < Y\max \le Y3$,

$$Cdil = \max\,[C11, C8 + C9 * XD + C10 * XD^2] * (Y3 - Y\max)/(Y3 - Y2) + \max\,[0.0, C12 + C13 * XD] * (Y\max - Y2)/(Y3 - Y2)$$

If $Y3 < Y\max \le 1$,

$$Cdil = \max\,[0.0, C12 + C13 * XD]$$

where

$$Y\max = XH2 + (XH2CC / XCOCC) * XCO$$
$$XD = XH2O + XCO2$$
$$Ci = C2200(i)$$
$$Yi = C2200(13 + i)$$

The values of C2200(i) are sensitivity coefficients as described below:

(1) - Constant in base flame speed correlation.
(default = 59.2, units = m/s, equiv = none)

(2) - Constant in base flame speed correlation.
(default = 1.792, units = m/s, equiv = none)

(3) - Constant in base flame speed correlation.
(default = 9.576, units = m/s, equiv = none)

(4) - Constant in base flame speed correlation.
(default = 15., units = m/s, equiv = none)

(5) - Constant in base flame speed correlation.
(default = 45., units = m/s, equiv = none)

(6) - Constant in base flame speed correlation.
(default = 55., units = m/s, equiv = none)

(7) - Constant in base flame speed correlation.
(default = 48.58, units = m/s, equiv = none)

(8) - Constant for flame speed diluent effect.
(default = 1.0, units = none, equiv = none)

(9) - Constant for flame speed diluent effect.
(default = -4.53, units = none, equiv = none)

(10) - Constant for flame speed diluent effect.
(default = 5.37, units = none, equiv = none)

(11) - Constant for flame speed diluent effect.
(default = 0.05, units = none, equiv = none)

(12) - Constant for flame speed diluent effect.
(default = 1.0, units = none, equiv = none)

(13) - Constant for flame speed diluent effect.
(default = -1.29, units = none, equiv = none)

(14) - Range limit for flame speed correlation.
(default = 0.1, units = none, equiv = none)

(15) - Range limit for flame speed correlation.
(default = 0.2, units = none, equiv = none)

(16) - Range limit for flame speed correlation.
(default = 0.3, units = none, equiv = none)

(17) - Range limit for flame speed correlation.
(default = 0.4, units = none, equiv = none)

(18) - Range limit for flame speed correlation.
(default = 0.6, units = none, equiv = none)

C2201 - Maximum Overshoot of Ignition Limit

A time advancement is vetoed and repeated with a smaller timestep if either the combustible fraction overshoots the ignition limit excessively while flammable or if the diluent or oxygen concentration overshoots the deinerting limit excessively while the combustible concentration is above the ignition limit.

(1) - Overshoot allowed on combustible gas concentration.
(default = 0.005, units = none, equiv = TEST1)

(2) - Overshoot allowed on deinerting limit (O_2 or CO_2 + H_2O).
(default = 0.01, units = none, equiv = TEST2)

C2202 - Combustion Completeness Parameters

The default combustion completeness (CC) is evaluated as follows

$$CC = 1 - Y\min/Y\max \qquad \text{(CC constrained such that } 01 \le CC \le 1\text{)}$$

where for Ymax ≤ C2202(2):

$$Y\min/Y\max = C2202(1)$$

and for Ymax > C2202(2):

$$Y\min/Y\max = C2202(1) - C2202(3)\,(Y\max - C2202(2))$$

Ymax is LeChatelier's parameter (described above) at the start of the burn, Ymin is LeChatelier's parameter at the end of the burn, and the values of C2202(i) are sensitivity coefficients as described below.

(1) - Slope of combustion completeness correlation for low combustible gas concentrations.
(default = 1.0, units = none, equiv = none)

(2) - Combustible gas concentration where slope of combustion completeness correlation changes.
(default = 0.03746, units = none, equiv = none)

(3) - Multiplier for combustion completeness correlation at high combustible gas concentration.
(default = 23.4116, units = none, equiv = none)

C2203 - Minimum Debris Temperature to Invoke DCH Parameters

If the temperature of the airborne debris in a control volume falls below this value, then ignition limits and flame speed and combustion completeness correlations will revert to their non-DCH values.

(1) - Minimum airborne debris temperature for DCH parameters.
(default = 600., units = K, equiv = none).

4. Plot Keys and Control Function Variables

The plot keys (/p/) and control function argument (/c/) are described below.

BUR-CPUC	/p/	CPU time used by the calculation routines in the BUR package. (units = s)
BUR-CPUE	/p/	CPU time used by the edit routines in the BUR package. (units = s)
BUR-CPUR	/p/	CPU time used by the restart routines in the BUR package. (units = s)
BUR-CPUT	/p/	Total CPU time used by the calculational, edit, and restart routines of the BUR package. (units = s)
BUR-N-SE.n	/p/	Number of times a burn has started or ended in control volume n. It is odd if a burn is occurring in the volume, and even if no burn is occurring. (units = none)
BUR-LOG	/c/	Logical control function argument that is TRUE if any control volume is burning and FALSE otherwise. (type = logical, units = none)
BUR-O2-RAT.n	/cp/	The rate of oxygen consumption from burning in CVH volume n. (units = kg/s)
BUR-02-TOT.n	/cp/	The total amount of oxygen consumed by burning in CVH volume n. (units = kg)

BUR-H2-RAT.n	/cp/	The rate of hydrogen consumed from burning in CVH volume n. (units = kg/s)
BUR-H2-TOT.n	/cp/	The total amount of hydrogen consumed by burning in CVH volume n. (units = kg)
BUR-CO-RAT.n	/cp/	The rate of carbon monoxide consumption from burning in CVH volume n. (units = kg/s)
BUR-CO-TOT.n	/cp/	The total amount of carbon monoxide consumed by burning in CVH volume n. (units = kg)
BUR-H2O-RAT.n	/cp/	The rate of steam production from burning in CVH volume n. (units = kg/s)
BUR-H2O-TOT.n	/cp/	The total amount of steam produced by burning in CVH volume n. (units = kg)
BUR-CO2-RAT.n	/cp/	The rate of carbon dioxide production from burning in CVH volume n. (units = kg/s)
BUR-CO2-TOT.n	/cp/	The total amount of carbon dioxide produced by burning in CVH volume n. (units = kg)
BUR-POWER.n	/cp/	The power generated by burning in CVH volume n. (units = W)
BUR-ENERGY.n	/cp/	The energy produced by burning in CVH volume n. (units = J)
BUR-O2-FTOT.n	/p/	Total oxygen burned in flow path n. (units = kg)
BUR-H2-FTOT.n	/p/	Total hydrogen burned in flow path n. (units = kg)

BUR-D2-FTOT.n	/p/	Total deuterium burned in flow path n. (units = kg)
BUR-CO-FTOT.n	/p/	Total carbon monoxide burned in flow path n. (units = kg)
BUR-H2O-FTOT.n	/p/	Total steam produced in flow path n. (units = kg)
BUR-CO2-FTOT.n	/p/	Total carbon dioxide produced in flow path n. (units = kg)
BUR-FENERGY.n	/p/	Total energy produced in flow path n.

5. Illustrative Input

The illustrative input for the BUR package is a four-volume problem. The inputs for MELGEN and MELCOR are given below. Only the parameters for burn rate, propagation speed, and timestep control are changed from the defaults for this problem.

5.1 MELGEN Input

```
TITLE ...
JOBID ...
*
* NONCONDENSIBLE GAS INPUT
*
NCG001  H2
NCG002  O2
NCG003  CO2
NCG004  CO
*
* CONTROL VOLUME SETUP ...
*
* FLOW PATH INPUT ...
*
* BURN PACKAGE INPUT
*
BUR000  0   * ACTIVATE BURN PACKAGE
*
* INPUT BURN RATE AND PROPAGATION SPEED PARAMETERS
*
```

```
BUR100  4  0  10.  .7
BUR101  7  1  20.  .5
BUR102  8  1  25.  .6
BUR103  9  0   8.  .1
```

5.2 MELCOR Input

```
TITLE ...
JOBID ...
RESTART ...
*
* OTHER INPUT
*
* BURN Timestep INPUT
*
BURTIM,  -.15
```

6. Discussion of Output

In the regular edits in MELGEN and MELCOR, most of the output is self-explanatory and directly reflects user input. For each MELCOR edit, the volumes that are burning or are inert are summarized. In addition, burning volumes are indicated at every timestep regardless of whether an edit is appropriate. An area that requires further explanation, however, is the node connectivity table for burn propagation. In that table, the orientation is given as -1, 0, or 1. These values represent downward, horizontal, and upward propagation directions and are determined from the user input values of the flow path elevations.

Messages are written to the output file and the special message file for a detonation, the start and end of a deflagration, and for propagation. The ID's are

BUR001 - Detonation
BUR002 - Deflagration has started
BUR003 - Propagation
BUR004 - Deflagration has ended

The message lists the time as well as the applicable volumes. These messages are written to the files regardless of whether an edit was desired or not. In addition, when the appropriate input is specified on record BUR004, a plot dump is requested at the same time the message is written out.

7. Error Messages

The error messages in MELGEN pertain to the input and are self-explanatory. The only error messages in MELCOR for the BUR package reflect errors returned from calls to the control function package.