Consequence Analysis of Li-Ion Battery Thermal Runaway Events with Chemical Equilibrium Analyses

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Motivation

The current approach to toxic gas hazards during LIB thermal runaway is expensive and not 'a priori'

Problem Statement:

Toxic gas release during thermal runaway of Li-ion batteries is a potential hazard, but is not well characterized

Current Approach: Experimental evaluation of single batteries

Objectives:
1) Develop an a priori modeling approach
2) Validate against existing experimental data
3) Apply to various LIB designs and conditions

Overview of Chemical Equilibrium Analysis (CEA)

CEA is utilized to predict reaction equilibrium conditions

Input Parameters

1) Cell Composition
- Anode, Cathode, Electrolyte, etc.
- Mass concentration and ΔH_f^0

2) Ambient Conditions
- Pressure (ambient vs. vacuum)
- Gas composition (air, ISS, or vacuum)

Output Parameters

1) Combustion Chemistry
- Relative product concentrations
- Product phase (condensed vs. gaseous)

2) Flame Temperature

3) Total Heat Release

T_{AF}
P_c

LIB Combustion

LNNL Cheetah 8.0

Thermodynamic Libraries

Minimization of Gibbs Energy

$$G = H - Ts$$
$$\Delta G = \Delta G^0 + RTlnQ$$
$$\Delta G^0 = -RTlnK_p$$
$$\left(\frac{\partial lnK}{\partial T}\right)_P = \frac{\Delta H^0}{RT^2} \;\&\; \left(\frac{\partial lnK}{\partial P}\right)_T = \frac{\Delta V^0}{RT^2}$$

[Gordon and McBride, 1996]

Literature Review:

Experimental Approaches

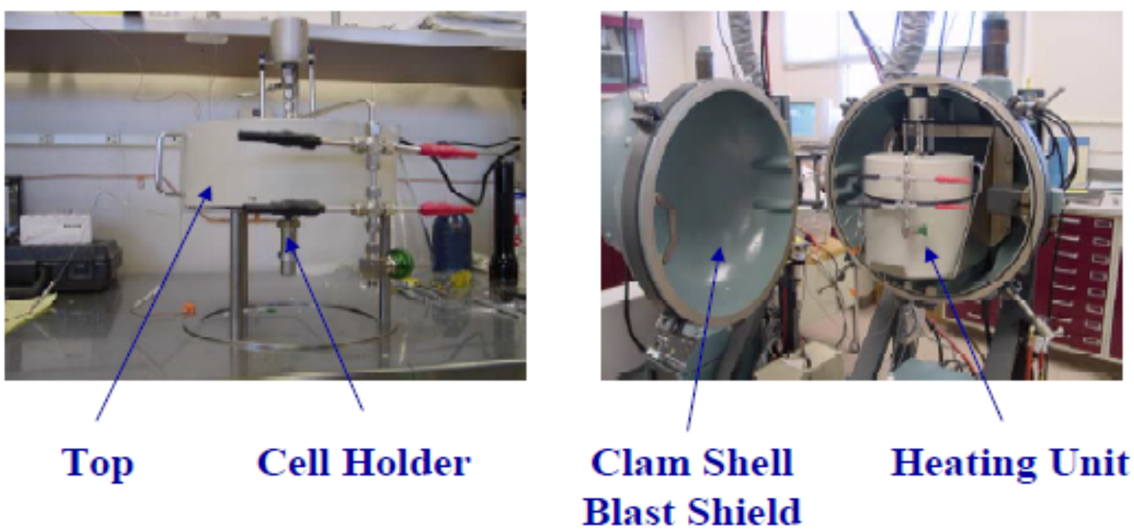
State-of-the-Art Experiments

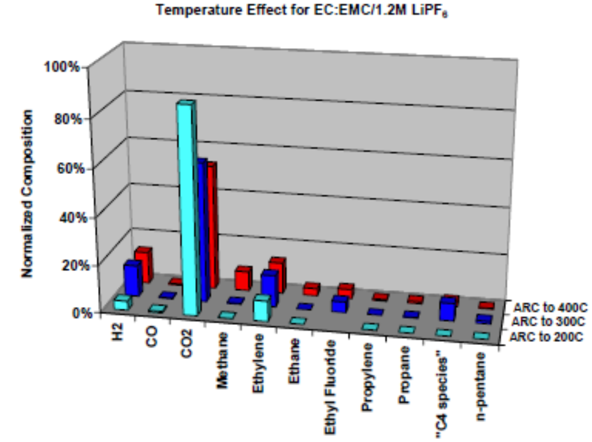
ARC and reaction gas composition analysis

Experiments
- DSC, ARC with temperature-transient gas sampling
- Reaction Gas Sampling (GC, FTIR)
- Cell-level and sub-components

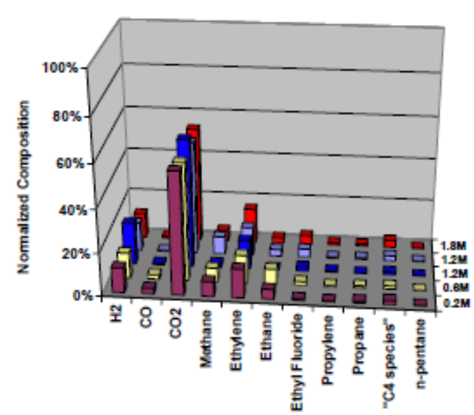
Shortcomings
- No ‘true’ ignition and combustion (slow dT/dt)
- Gas sampling data may be useful for kinetics modeling

Gen1 Cells: (Argonne National Laboratory Design)	Anode:	75% MCMB-6-2800 Carbon 16% SFG-6 Graphite 9% PVDF Binder
	Cathode:	84% $LiNi_{0.85}Co_{0.15}O_2$ 4% Carbon Black, 4% SFG6 Graphite 8% PVDF Binder
	Electrolyte:	1M $LiPF_6$ in EC:DEC (1:1)
Gen2 Cells: (Argonne National Laboratory design)	Anode:	92% MAG10 Graphite 8% PVDF Binder
	Cathode:	84% $LiNi_{0.80}Co_{0.15}Al_{0.05}O_2$ 4% Carbon Black, 4% SFG6 Graphite 8% PVDF Binder
	Electrolyte:	1.2M $LiPF_6$ in EC:EMC (3:7)





EC:EMC/LiPF$_6$: Normalized Gas Composition with Increasing LiPF$_6$ (400C)



Sandia National Labs; [Roth et al., 2004]

State-of-the-Art Experiments

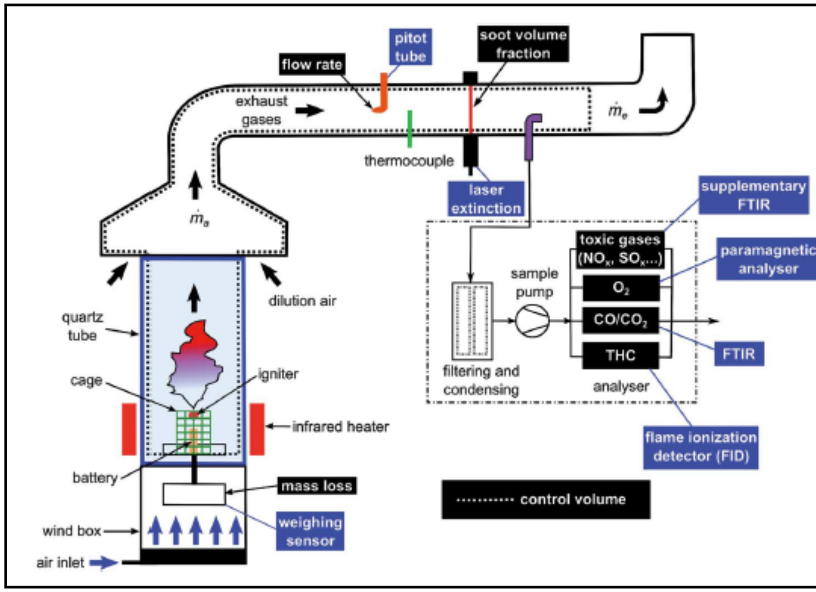
Cone calorimetry and *reaction gas composition* *analysis*

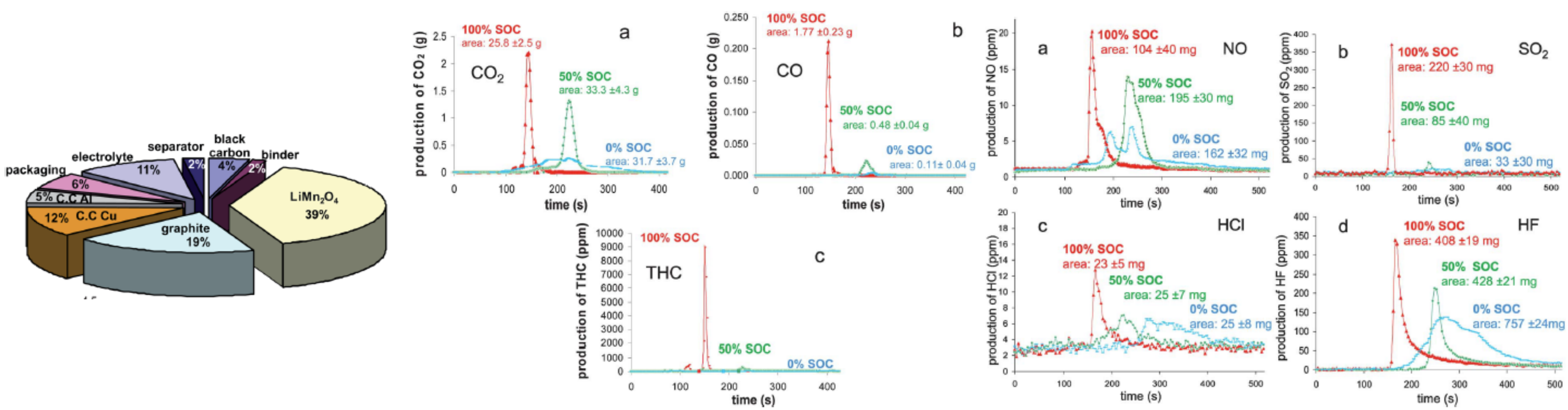
Experiments

- Cone Calorimetry (Heat Release Rate)
- Reaction Gas Sampling (Reaction Composition)

Shortcomings

- Cell composition not well defined
  - Numerous estimates
  - Electrolyte, salt, SEI
- Oxidizer volume is not well quantified





[Ribiere et al., 2012]

State-of-the-Art Experiments

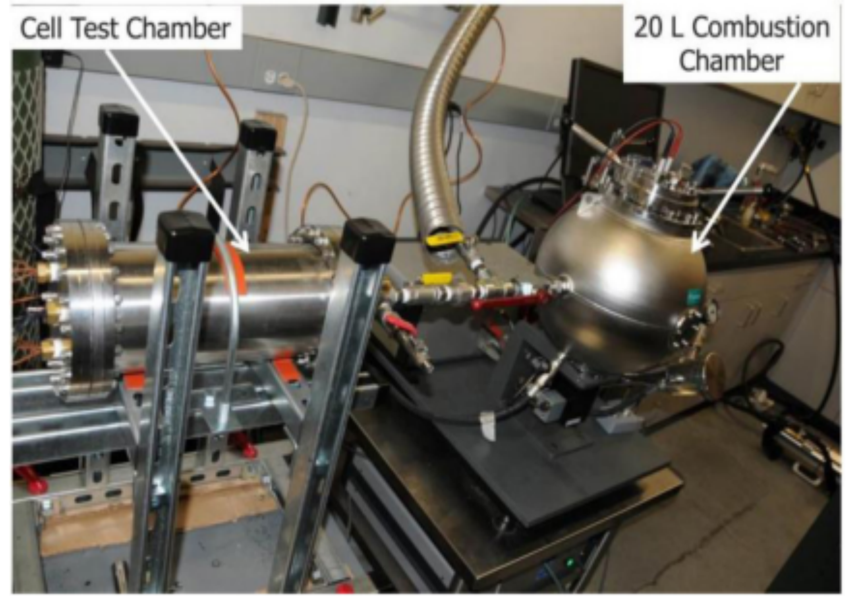
CV 'bomb' with gas collection and explosion analysis

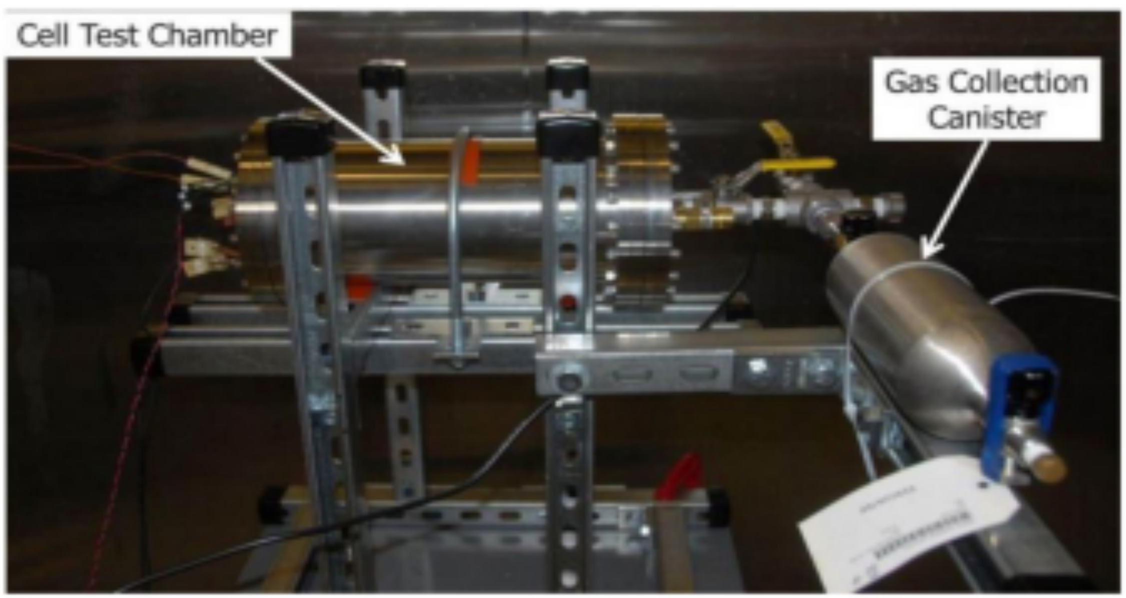
Experiments

- Constant-Volume (CV) Vessel with TR
- Reaction Gas Collection and Explosion
- Atmosphere Control

Shortcomings

- Cell composition not fully characterized
    - Lithium salts, SEI not included
- Slow Heating Rates (~1 K/s)





Cell Composition

Component	Chemical Compound	Molecular Formula	ΔH_c ($kJ.g^{-1}$)	Mass %
Tape	Polyester Terephthalate	$(C_{10}H_8O_4)_n$	22.00 [25]	0.2%
Label	Polypropylene	$(C_3H_6)_n$	42.66 [24]	0.5 %
Separator	Polypropylene[1]	$(C_3H_6)_n$	42.66 [24]	6.4%
Electrolyte w/o Salt	See Table 2.		19.31[(*)]	9.5%
Outer Packaging (Top)	Nylon 6	$(C_6H_{11}NO)_n$	28.74 [25]	2.2%
Outer Packaging (Bottom)	Polypropylene	$(C_3H_6)_n$	42.66 [24]	2.1%
Positive Tab	Polyester Terephthalate	$(C_{10}H_8O_4)_n$	22.00 [25]	0.9%
Negative Tab	Polyester Terephthalate	$(C_{10}H_8O_4)_n$	22.00 [25]	0.9%
$LiCoO_2$ coated, positive electrode (aluminum)	Lithium Cobalt Oxide	$LiCoO_2$	Inorganic Material	42.4%
Graphite-coated negative electrode (copper)	Lithium-intercalated Graphite (charged)	LiC_6	Inorganic Material	34.9%

Chemical Compound	Molecular Formula	ΔH_c ($kJ.g^{-1}$)	% Volume in Electrolyte	% Mass in Electrolyte
Ethylene Carbonate	$C_3H_4O_3$	12.30 [26]	15.1	12
Dimethyl Carbonate	$C_3H_6O_3$	13.40 [27]	3.1	3
Diethyl Carbonate	$C_5H_{10}O_3$	21.15 [26]	70.8	76
Propylene Carbonate	$C_4H_6O_3$	16.53 [26]	9.8	9

Vent Gas Composition

Gas	50% SOC (%vol)	100% SOC (%vol)	150% SOC (%vol)	Roth *et al.*[4] (%vol) Test 1/Test 2
Carbon Dioxide	32	30	20.9	61.4/75.8
Carbon Monoxide	3.61	22.9	24.5	15.1/6.4
Hydrogen	30	27.7	29.7	5.1/5.9
Total Hydrocarbons	34	19.3	24	---
Methane	5.78	6.39	8.21	7.4/1.9

Gas	50% SOC (%vol)	100% SOC (%vol)	150% SOC (%vol)
Methane	5.78	6.39	8.21
Ethylene	5.57	2.19	10.77
Ethane	2.75	1.16	1.32
Propylene	8.16	4.52	0.01
Propane	0.68	0.26	2.54
Isobutane	0.41	0.20	0.13
n-Butane	0.67	0.56	0.39
Butenes	2.55	1.58	0.60
Isopentane	0.45	0.07	0.04
n-Pentane	1.94	0.73	0.30
Benzene	0.14	0.11	0.33
Toluene	0.06	0.02	0.05
Ethylbenzene	0.01	0.00	0.00
m+p Xylenes	0.01	0.00	0.00

Exponent, Inc.; [Somandepalli et al., 2014]; [Somandepalli and Biteau, 2014]

State-of-the-Art Experiments

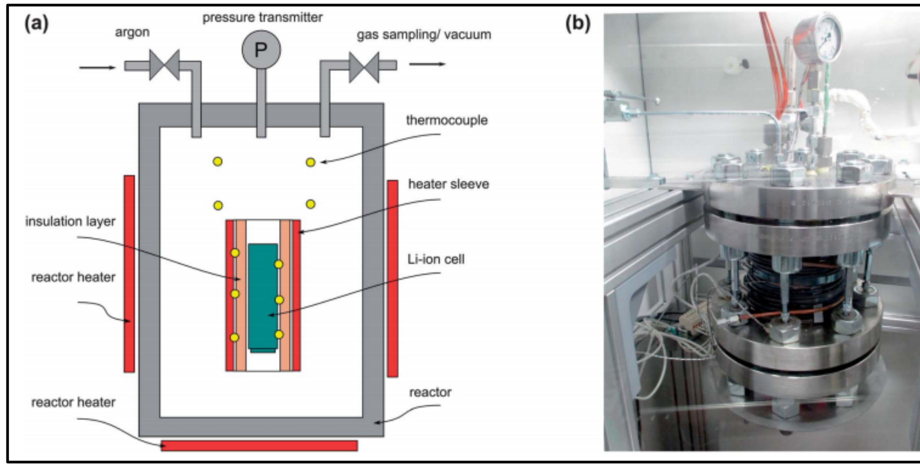
CV 'bomb' with reaction gas analysis

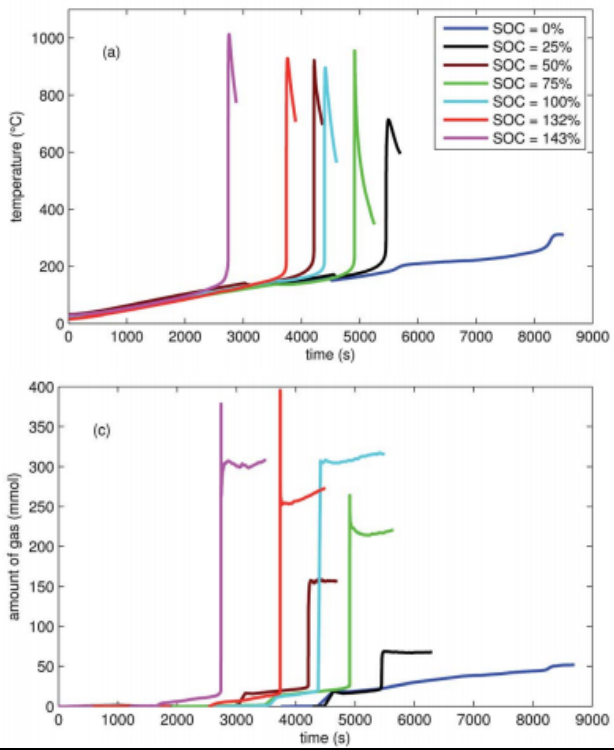
<u>Experiments</u>

- CV Vessel with Gas Sampling (GC)
- Full cell composition given (NCA & LFP)

<u>Shortcomings</u>

- Cell compositions contain some uncertainty
- Slow heating rates (~0.1 K/min)





No.	Cell	SOC (%)	θ_R (°C)	θ_m (°C)	Δm (g)	n_{sum}^{ideal} (mmol)	H_2 (%)	CO_2 (%)	CO (%)	CH_4 (%)	C_2H_4 (%)	C_2H_6 (%)
1	NCA	0	—	302	—	65	1.7	94.6	1.6	1.6	0.3	—
2	NCA	0	160	316	4.4	52	1.8	94.7	1.9	1.2	0.4	—
3	NCA	0	160	315	4.5	55	1.2	96	1.5	1.1	0.2	—
4	NCA	0	161	214	4.4	39	0.9	96.2	1.1	1.4	0.3	—
5	NCA	0	150	243	4.4	59	0.8	96.6	1	1.3	0.3	—
6	NCA	25	150	739	5.9	67	15.5	62.7	5.5	8.7	7.5	—
7	NCA	50	140	970	8.5	157	17.5	33.8	39.9	5.2	3.2	0.4
8	NCA	75	140	955	—	217	24.2	20.8	43.7	7.5	3.3	0.5
9	NCA	100	144	904	—	273	22.6	19.7	48.9	6.6	2.4	—
10	NCA	100	138	896	20.5	314	26.1	17.5	44	8.9	2.7	0.9
11	NCA	100	136	933	20.9	244	28.5	22.7	41.5	5.9	1.3	0.3
12	NCA	112	144	—	19.2	252	25.1	18.8	48.1	5.9	2.1	—
13	NCA	120	80	929	—	281	23.5	20.8	48.7	5.4	1.6	—
14	NCA	127	80	983	—	317	28.8	16.2	46.6	6.4	1.3	0.3
15	NCA	132	80	943	17	262	25.8	18.9	49.2	4.7	1.4	—
16	NCA	143	65	1075	20.1	303	26.2	22	43.4	6.9	1.5	—
17	LFP	0	—	251	6.1	55	2.7	93.5	1.8	0.7	0.7	0.7
18	LFP	25	195	231	6.1	31	7.1	85.3	3.1	1.2	3.1	0.2
19	LFP	50	130	283	6.1	32	20.8	66.2	4.8	1.6	6.6	—
20	LFP	75	149	362	6.3	41	21.8	62.6	6.4	1.9	6.3	1
21	LFP	100	140	440	7.1	32	29.4	48.3	9.1	5.4	7.2	0.5
22	LFP	115	155	395	6.2	61	34	52.2	6.4	2.6	4.7	0.1
23	LFP	130	80	448	—	58	30.1	55.8	7.7	6.4	—	—

[Golubkov et al., 2014]; [Golubkov et al., 2015]

State-of-the-Art Experiments

CV 'bomb' with reaction gas analysis

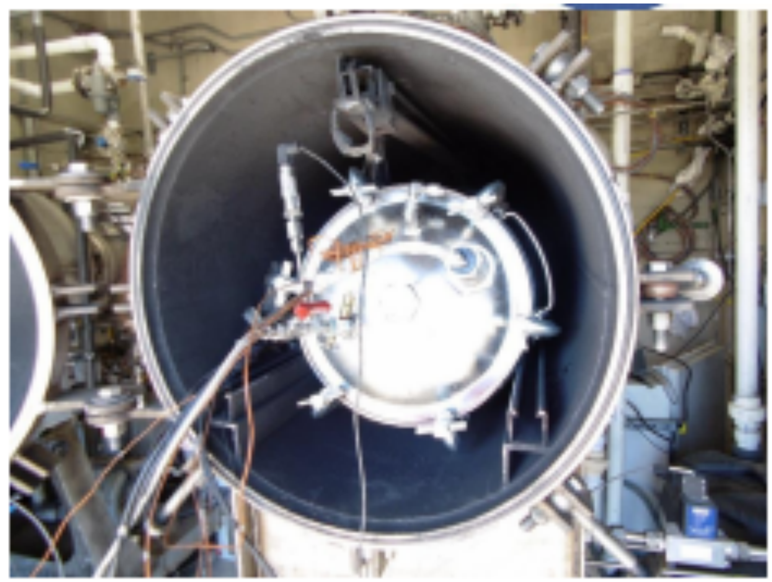
<u>Experiments</u>

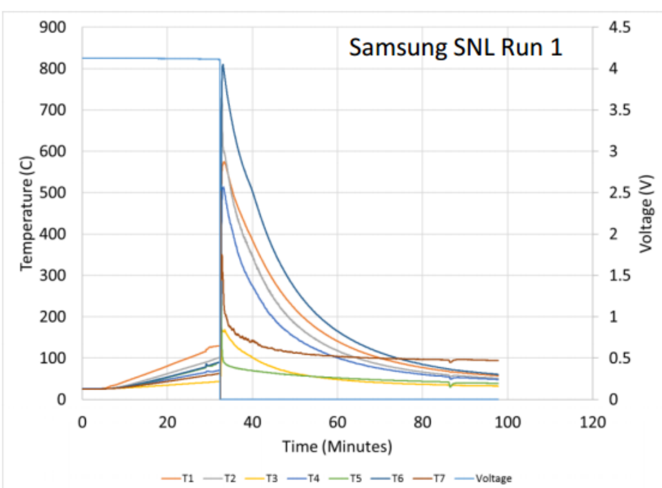
- CV Vessel TR with Gas Analysis (GC), CCP Analysis
- Atmosphere Control
- Commercial 18650 Cells

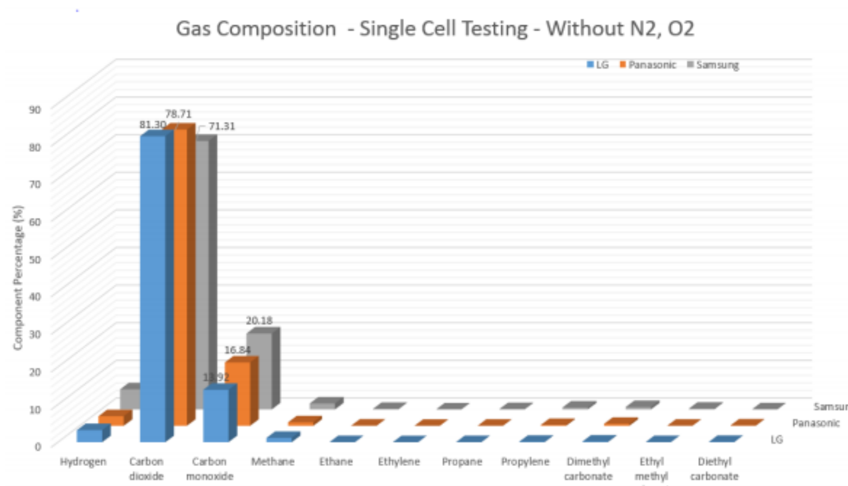
Manufacturer	Cell (18650)	Chemistry	Capacity (Ah)
Samsung	ICR-26F	$LiCoO_2$ (LCO)	2.6
LG	INR-MJ1	$LiNiMnCoO_2$ (NMC)	3.5
Panasonic	NCR-B	$LiNiCoAlO_2$ (NCA)	3.4

<u>Shortcomings</u>

- Cell composition not well defined (proprietary)
- Slow heating rates (~0.1 K/s)







[Delafuente, 2018]

Literature Summary

Toxic product formation in LIB thermal runaway is an active area of research

<u>*Summary:*</u>

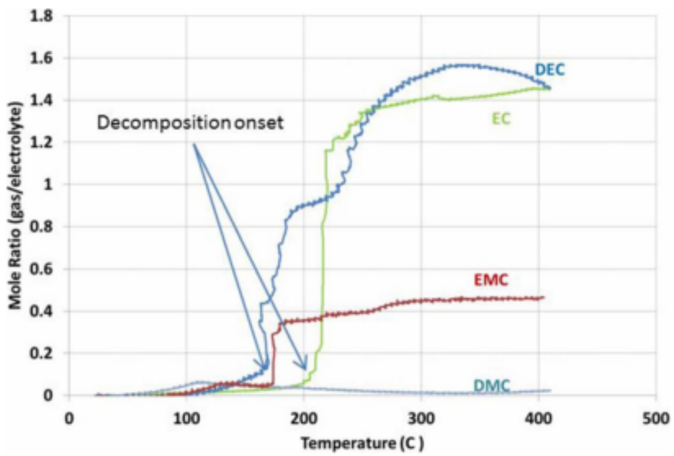
- Toxic gas release during LIB thermal runaway is a noteworthy hazard and an active are of research
- Several experimental approaches are currently being taken
  - ARC, cone calorimetry, closed vessel sampling
  - Current experimental data lacks 'accurate' cell compositions
  - Temperature ramp (dT/dt) is typically too slow
  - Very little modeling has been completed
  - [Golubkov et al., 2015] experiments are the best available

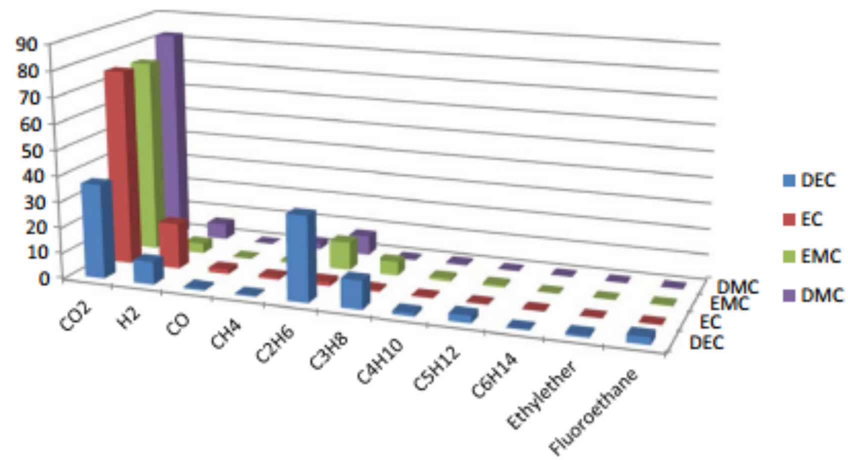
CEA Modeling – Electrolyte Solutions

Electrolyte Compositional Analysis

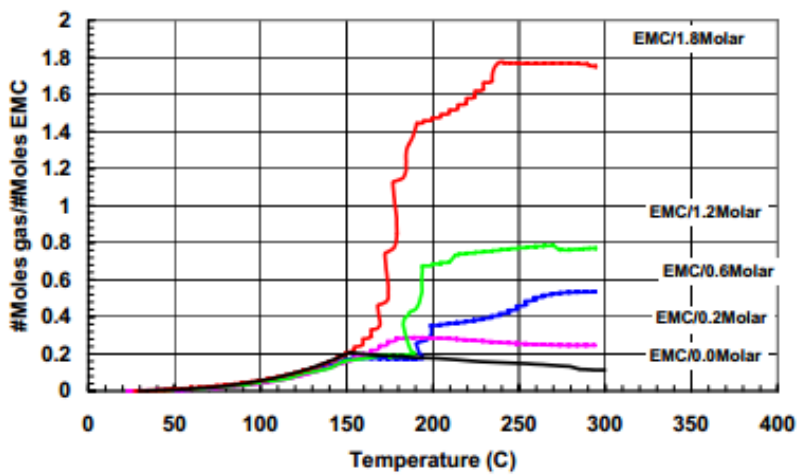
Electrolyte reaction data provided by Sandia National Labs

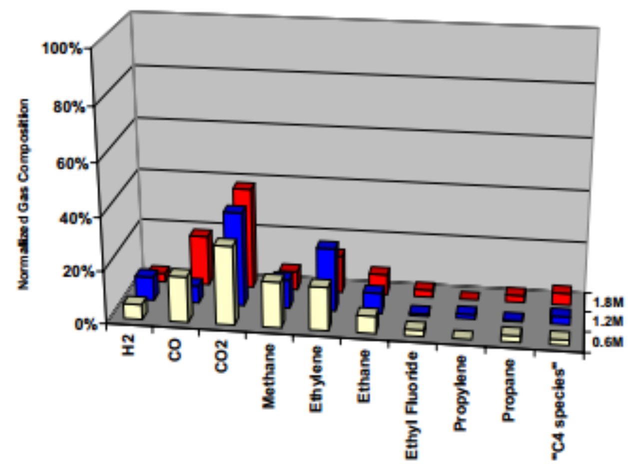
1.2 M $LiPF_6$ in various electrolytes (DEC, EC, EMC, DMC)





Various concentrations of $LiPF_6$ in EC





Sandia National Labs; [Roth et al., 2004]

Electrolyte Compositional Analysis

Empirical density correlations developed

CEA inputs require knowledge of relative mass fractions (not concentration)

Mass Fraction Computation

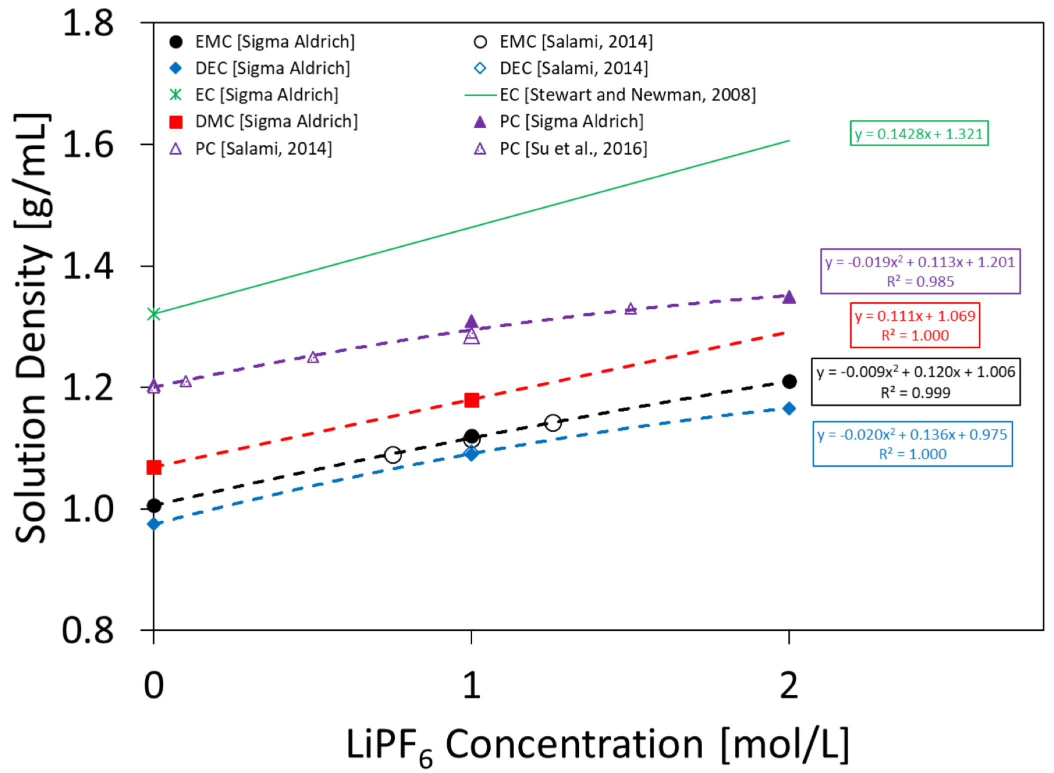
$$Y_i = C_i \frac{M_i}{\rho_{sol}}$$

Y_i – component mass fraction

C_i – component concentration [mol/L]

M_i – component molecular weight [g/mol]

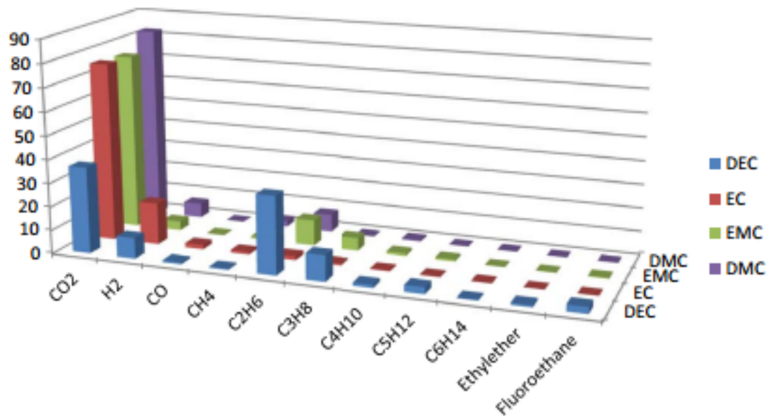
ρ_{sol} – solution density [g/L]

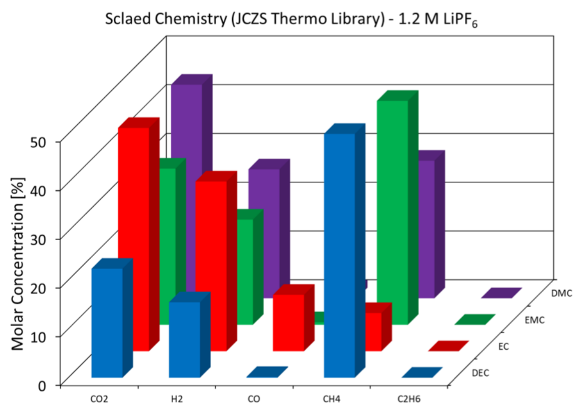


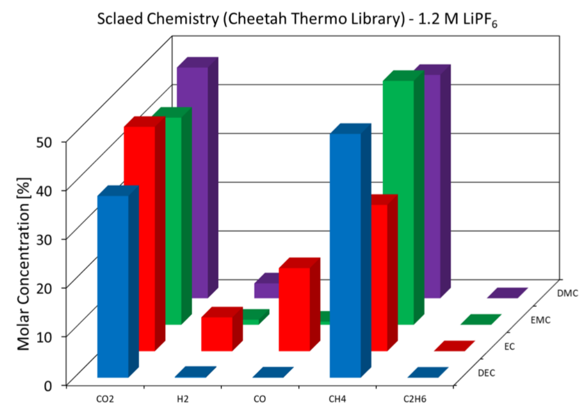
CEA Analysis – 1.2 M $LiPF_6$ in DEC, EC, EMC, DMC

Moderate agreement between experiment and computation

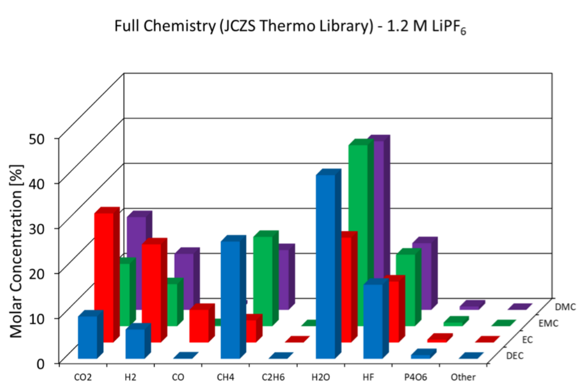
Scaled Chemistry

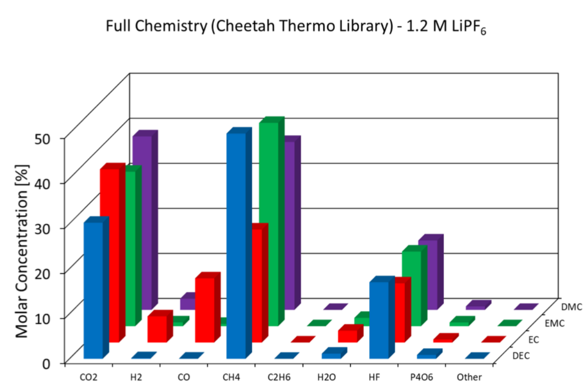


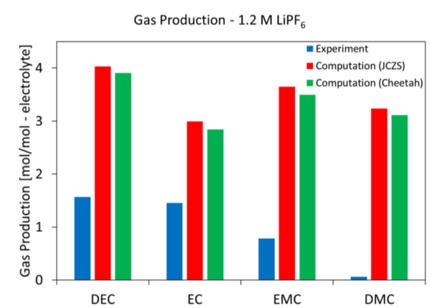


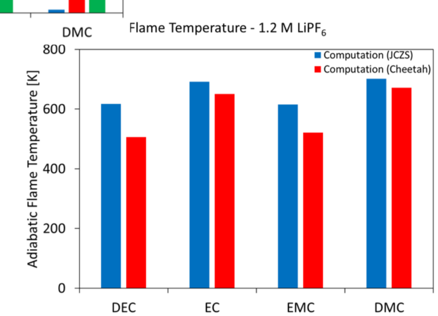


Full Chemistry







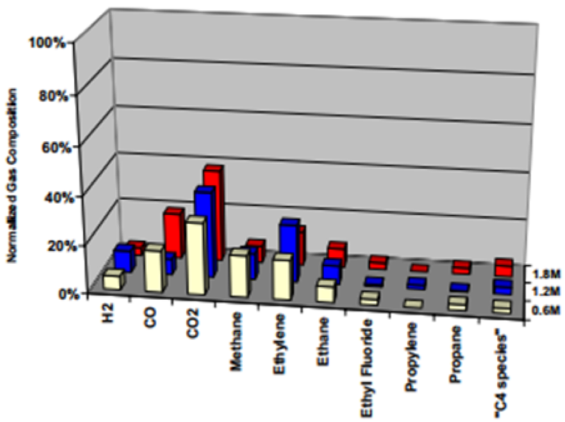


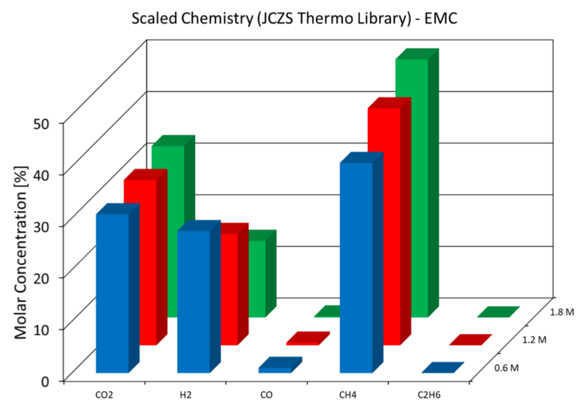
Sandia National Labs; [Roth et al., 2004]

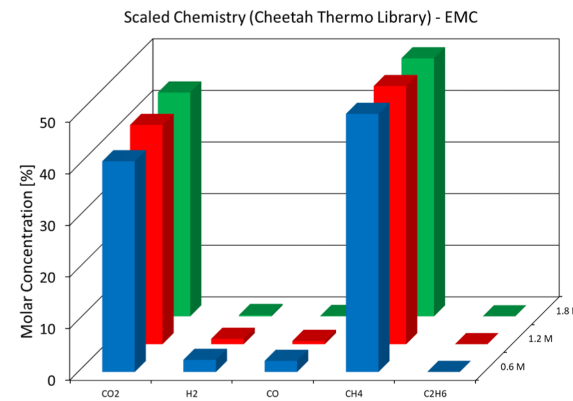
CEA Analysis – $LiPF_6$ in EC

Moderate agreement ***between experiment and computation***

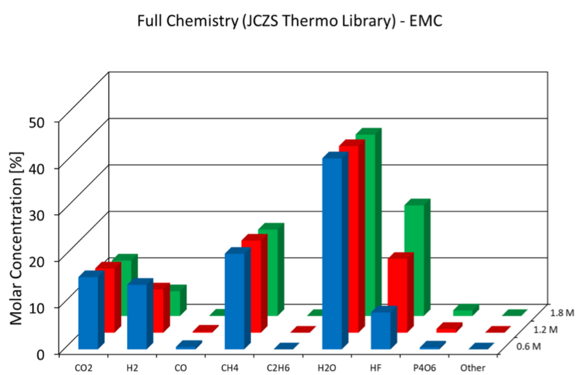
Scaled Chemistry

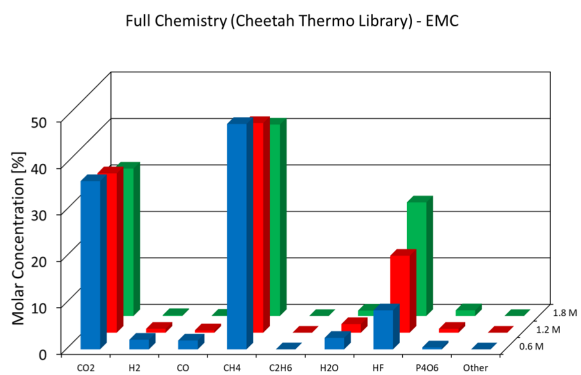


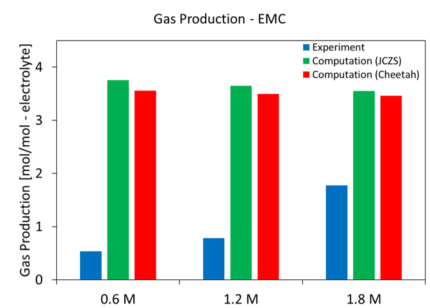


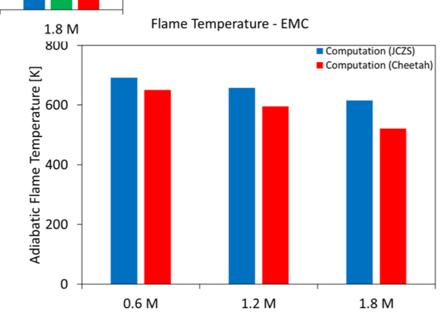


Full Chemistry









Sandia National Labs; [Roth et al., 2004]

CEA Analysis – Electrolyte Solutions

Key Findings:

- Experimental and Computational Agreement
  - Moderate (chemistry) and Poor (total gas production)
  - May be due to slow heating conditions

- Thermodynamic libraries yield significantly different results
  - JCZS library favors H_2 and H_2O production
  - Cheetah library favors CH_4 production
  - Cheetah library agreed better with experiments

- Appreciable amounts of toxic substances detected (HF and P_4O_6)
  - Dilute compounds not yet evaluated

CEA Modeling – Lithium Ion Battery

Battery Compositional Analysis

Estimated battery composition given by Golubkov et al.

Experimental Methods:

- Mass and geometry of main components directly measured
  - Anode, cathode, separator, electrolyte
- Anode and cathode chemistry
  - Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES)
  - Scanning Electron Microscopy (SEM)
  - Energy Dispersive X-Ray (EDX) Analysis
- Electrolyte identification
  - Solution immersion (CH_2Cl_2)
  - Gas Chromatography Mass Spectrometry (GC-MS)
- Separator Identification
  - Differential Scanning Calorimetry (DSC)
  - Thermal Gravimetric Analysis (TGA)

[Golubkov et al., 2014]; [Golubkov et al., 2015]

Battery Compositional Analysis

Estimated battery composition given by Golubkov et al.

Key Compositional Assumptions:

- Binder chemistry and composition
  - Anode: 5% of total coating, Na-carboxymethylcellulose (Na-CMC, S=0.7)
    - Conducting agent: 5% of total coating, carbon black
  - Cathode: 5% of total coating, polyvinylidene fluoride (PVDF)

- Electrolyte salt
  - $LiPF_6$ at a concentration of 1.1 mol/L
  - 2% vinylene carbonate (VC, $C_3H_2O_3$) for SEI improvement

- Solid electrolyte interphase (SEI)
  - Complete VC polymerization to poly(vinylene carbonate) $C_6H_4O_6$ {1:1}
  - Ethylene carbonate reduction: lithium ethylene dicarbonate $(CH_2OCO_2Li)_2$ {1:2}
    lithium carbonate Li_2CO_3 {1:4}
  - Formation of lithium fluoride LiF {1:4}

- Irreversible capacity loss
  - 8% of maximum anode capacity is trapped ($n_{Li}^{irr} = 0.08 n_{C_6}^{a}$)

[Golubkov et al., 2014]; [Golubkov et al., 2015]

Battery Compositional Analysis

ΔH_f^0 estimated from literature and computations

- LFP Battery composition is 'well' characterized
- Need heat of formation (ΔH_f^0) data for all components

	Component		Mass (g)	Mass (%)	Concentration (mol)	Concentration (%)
Cathode	Aluminum Foil	Al	2.14	7.53	0.079	16.61
	Active Material - LFP*	$LiFePO_4$	7.73	27.21	0.049	10.26
	Particle Coating	C	0.97	3.41	0.081	16.92
	Carbon Black	C	0.48	1.69	0.040	8.37
	Binder - Polyvinylidene Flouride (PVDF)	$(C_2H_2F_2)_n$	0.48	1.69	0.007	1.57
Anode	Copper Foil	Cu	3.86	13.59	0.061	12.72
	Active Material - Graphite*	LiC_6	4.84	17.04	0.061	12.83
	Binder - Sodium Carboxymethylcellulose (CMC)	$[C_6H_7O_2(OH)_{2.3}(OCH_2COONa)_{0.7}]_n$	0.26	0.92	0.001	0.25
	SEI - Lithium Flouride	LiF	0.02	0.07	0.001	0.16
	SEI - Lithium Carbonate	Li_2CO_3	0.06	0.21	0.001	0.17
Separator	Polypropylene (PP)	$(C_3H_6)_n$	0.76	2.68	0.018	3.78
	Polyehtylene (PE)	$(C_2H_4)_n$	0.39	1.37	0.014	2.91
Electrolyte	SEI - Polymer Organic - Poly(Vinylene Carbonate)	$(C_6H_4O_6)_n$	0.13	0.46	0.001	0.16
	SEI - Organic - Lithium Ethylene Dicarbonate	$(CH_2OCO_2Li)_2$	0.25	0.88	0.002	0.32
	Ethylene Carbonate (EC)	$C_3H_4O_3$	1.59	5.60	0.018	3.78
	Dimethyl Carbonate (DMC)	$C_3H_6O_3$	2.12	7.46	0.024	4.93
	Ethyl Methyl Carbonate (EMC)	$C_4H_8O_3$	1.06	3.73	0.010	2.13
	Propylene Carbonate (PC)	$C_4H_6O_3$	0.53	1.87	0.005	1.09
	Salt - Lithium Hexafluorophosphate	$LiPF_6$	0.74	2.60	0.005	1.02
*Mass and resultant properties dependent on state-of-charge (SoC); mass given at delithiated state (8% Li in anode)			28.41	100.00	0.477	100.00

Heat of Formation Data:

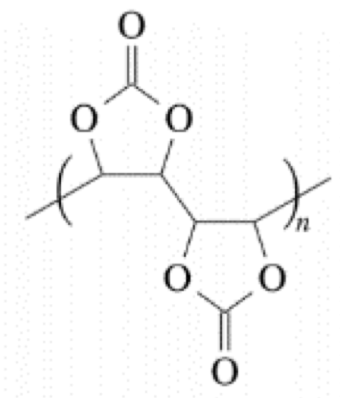
- Literature sources
  - Calorimetry
  - DFT computations
  - **NIST database**
- Additive group computations

[Golubkov et al., 2015]

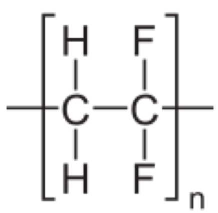
Heat of Formation Computations

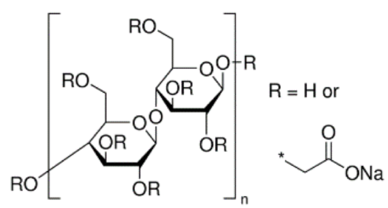
ΔH_f^0 *estimated from group additive methods*

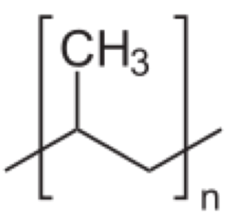
Example Calculation: Poly(Vinylene Carbonate) - $(C_6H_4O_6)_n$

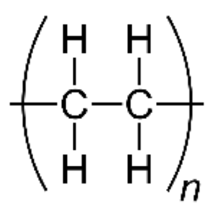


Group	Number	Group ΔH_f Contribution (kcal/mol)	Total Group ΔH_f Contribution (kcal/mol)	Total Group ΔH_f Contribution (kJ/mol)	ΔH_f (kJ/mol)
>C=O	2	-28.08	-56.16	-235.0	
-O-	4	-15.79	-63.16	-264.3	-617.88
>CH-	4	-0.705	-2.820	-11.80	
Ring Correction	2	-12.768	-25.536	-106.84	









Chemical		ΔH_f (kJ/mol)
Polyvinyidene Flouride (PVDF)	$(C_2H_2F_2)_n$	-390.93
Sodium Carboxymethylcellulose (CMC)	$[C_6H_7O_2(OH)_{2.3}(OCH_2COONa)_{0.7}]_n$	-1093.38
Polypropylene (PP)	$(C_3H_6)_n$	-62.93
Polyehtylene (PE)	$(C_2H_4)_n$	-43.46
Poly(Vinylene Carbonate)	$(C_6H_4O_6)_n$	-617.88

[Van Krevelen and Chermin, 1951]

CEA Inputs

Ambient gas (Ar) *evaluated by* *ideal gas law*

CEA Inputs:

- Battery composition
- Ambient conditions
  - Pressure ($P \sim 1\ atm$), Temperature ($T_0 = 298\ K$)
  - Gas composition and amount

Ambient Gas:

- Argon (Ar)

$$n = \frac{PV}{RT}$$

	Component		Molecular Weight	Mass		Concentration		Heat of Formation		Reference
			(g/mol)	(g)	(%)	(mol)	(%)	(kJ/mol)	(kJ/g)	
Cathode	Aluminum Foil	Al	26.982	2.14	7.53	0.079	16.61	0	0.00	-
	Active Material - LFP*	$LiFePO_4$	157.756	7.73	27.21	0.049	10.26	-1616.02	-10.24	[Iyer et al., 2006]
	Particle Coating	C	12.011	0.97	3.41	0.081	16.92	0	0.00	-
	Carbon Black	C	12.011	0.48	1.69	0.040	8.37	0	0.00	-
	Binder - Polyvinylidene Flouride (PVDF)	$(C_2H_2F_2)_n$	64.035	0.48	1.69	0.007	1.57	-390.93	-6.10	Calculated
Anode	Copper Foil	Cu	63.546	3.86	13.59	0.061	12.72	0	0.00	-
	Active Material - Graphite*	LiC_6	79.007	4.84	17.04	0.061	12.83	-11.65	-0.15	[Tanaka, 2014]
	Binder - Sodium Carboxymethylcellulose (CMC)	$[C_6H_7O_2(OH)_{2.3}(OCH_2COONa)_{0.7}]_n$	218.160	0.26	0.92	0.001	0.25	-1093.38	-5.01	Calculated
	SEI - Lithium Flouride	LiF	25.938	0.02	0.07	0.001	0.16	-616.93	-23.78	NIST
	SEI - Lithium Carbonate	Li_2CO_3	73.888	0.06	0.21	0.001	0.17	-1216.04	-16.46	NIST
Separator	Polypropylene (PP)	$(C_3H_6)_n$	42.080	0.76	2.68	0.018	3.78	-62.93	-1.50	Calculated
	Polyehtylene (PE)	$(C_2H_4)_n$	28.054	0.39	1.37	0.014	2.91	-43.46	-1.55	Calculated
Electrolyte	SEI - Polymer Organic - Poly(Vinylene Carbonate)	$(C_6H_4O_6)_n$	172.092	0.13	0.46	0.001	0.16	-617.88	-3.59	Calculated
	SEI - Organic - Lithium Ethylene Dicarbonate	$(CH_2OCO_2Li)_2$	161.946	0.25	0.88	0.002	0.32	-1513.2	-9.34	[Tanaka, 2014]
	Ethylene Carbonate (EC)	$C_3H_4O_3$	88.062	1.59	5.60	0.018	3.78	-531	-6.03	NIST
	Dimethyl Carbonate (DMC)	$C_3H_6O_3$	90.078	2.12	7.46	0.024	4.93	-608.76	-6.76	NIST
	Ethyl Methyl Carbonate (EMC)	$C_4H_8O_3$	104.105	1.06	3.73	0.010	2.13	-644	-6.19	NIST
	Propylene Carbonate (PC)	$C_4H_6O_3$	102.089	0.53	1.87	0.005	1.09	-614.1	-6.02	NIST
	Salt - Lithium Hexafluorophosphate	$LiPF_6$	151.905	0.74	2.60	0.005	1.02	-2296	-15.11	[Gavritchev et al., 2003]
				28.41	100.00	0.477	100.00			

*Mass and resultant properties dependent on state-of-charge (SoC); mass given at delithiated state (8% Li in anode)

Lithium Species Tracking

[Li] *species is defined through SoC linear approximation*

CEA inputs require knowledge of the apparent composition versus SOC (i.e. [*Li*] *atom accounting*)

$$(1-x)LiFePO_4 + xFePO_4$$

$$x = 1 - \left[\frac{n_{Li}^{irr} + n_{Li}^{res} + (1/F)\times SOC\times C^{nom}}{n_{LFP}^{a}}\right]$$

$$n_{Li}^{a} = n_{Li}^{res} + (1/F)\times SOC\times C^{nom}$$

$$n_{Li}^{irr} = 0.08 n_{C_6}^{a}$$

$$n_{Li}^{res} = (1/F)\times C^{res} = (1/F)\times 0.01 C^{nom}$$

x – Lithiation state of the cathode

n_{Li}^{irr} – [Li] trapped in anode during first charge (SEI formation)

n_{Li}^{res} – [Li] trapped in anode at full discharge

F – Faraday constant (96,485.3329 C/mol)

SOC – State-of-Charge (0 – 100%)

C^{nom} – Nominal cell capacity (A-h)

n_{LFP}^{a} – Amount of active cathode material

$n_{C_6}^{a}$ – Number of graphite units (C_6) in the anode

C^{res} – Residual capacity at full discharge (due to n_{Li}^{res})

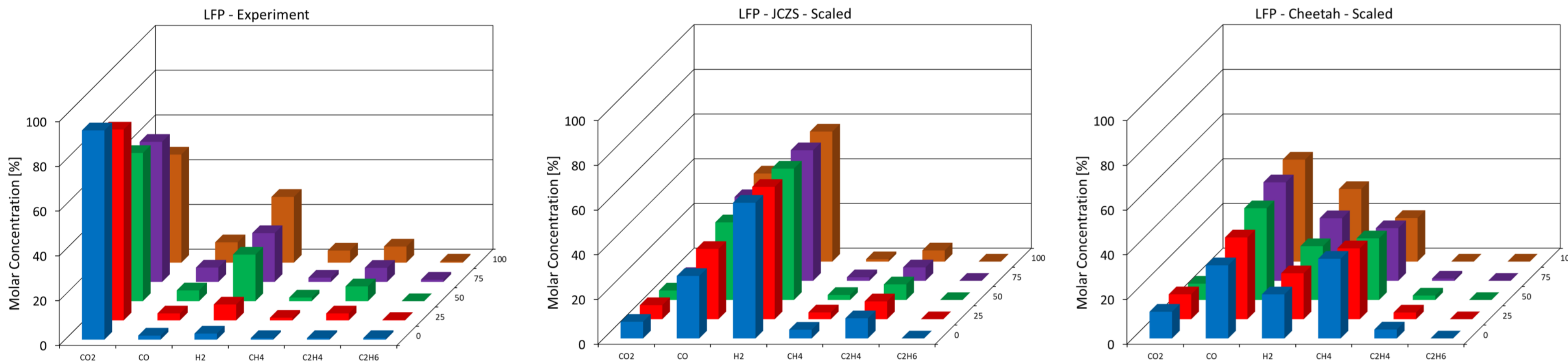
n_{Li}^{a} – [Li] in anode at SoC

[Golubkov et al., 2015]

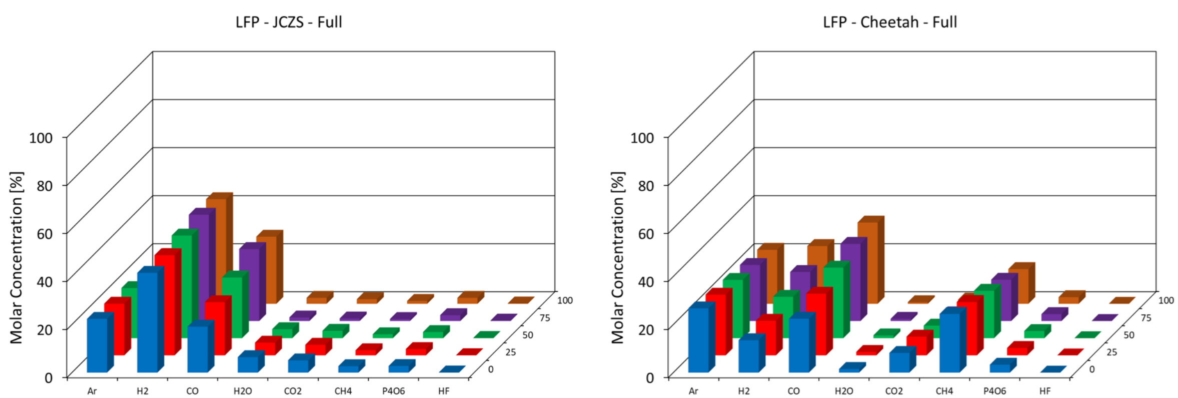
CEA Analysis – LFP Battery

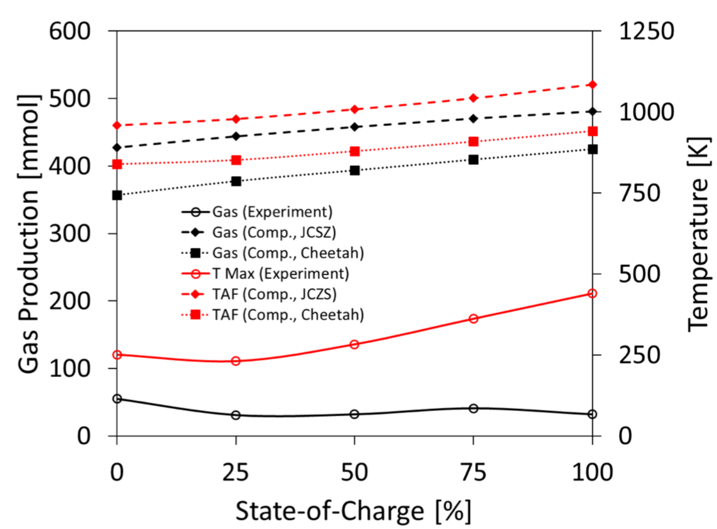
Moderate agreement between experiment and computation

Scaled Chemistry



Full Chemistry





[Golubkov et al., 2015]

CEA Analysis – LFP Battery

Key Findings:

- Experimental and Computational Agreement
  - Moderate (chemistry)
  - Poor (total gas production)
  - May be due to slow-heating experiments or unrestrictive LFP modeling

- Thermodynamic libraries yield significantly different results

- Appreciable amounts of toxic substances detected (HF and P_4O_6)
  - Dilute compounds not yet evaluated

Summary

- CEA modeling capability developed for TR of electrolytes and LFP batteries
  - Simple extension to other chemistries
  - Important computational products:
    - Product composition and chemistry
    - Flame temperature
    - Total heat release

- Experimental and computational agreement is moderate
  - Need for rapid heating experiments
  - Need for more restrictive modeling (cathode breakdown threshold)

- Future Work
  - Implementation of restrictive modeling inclusions
  - Validation via alternative cathode chemistry (NCA)
  - Validation via fast-heating experiments
  - Analyze effects of pressure, ambient composition, chemistry, etc.

Consequence Analysis of Li-Ion Battery Thermal Runaway Events with Chemical Equilibrium Analyses

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