The trouble with batteries:
Modelling electrochemical systems in a vehicle

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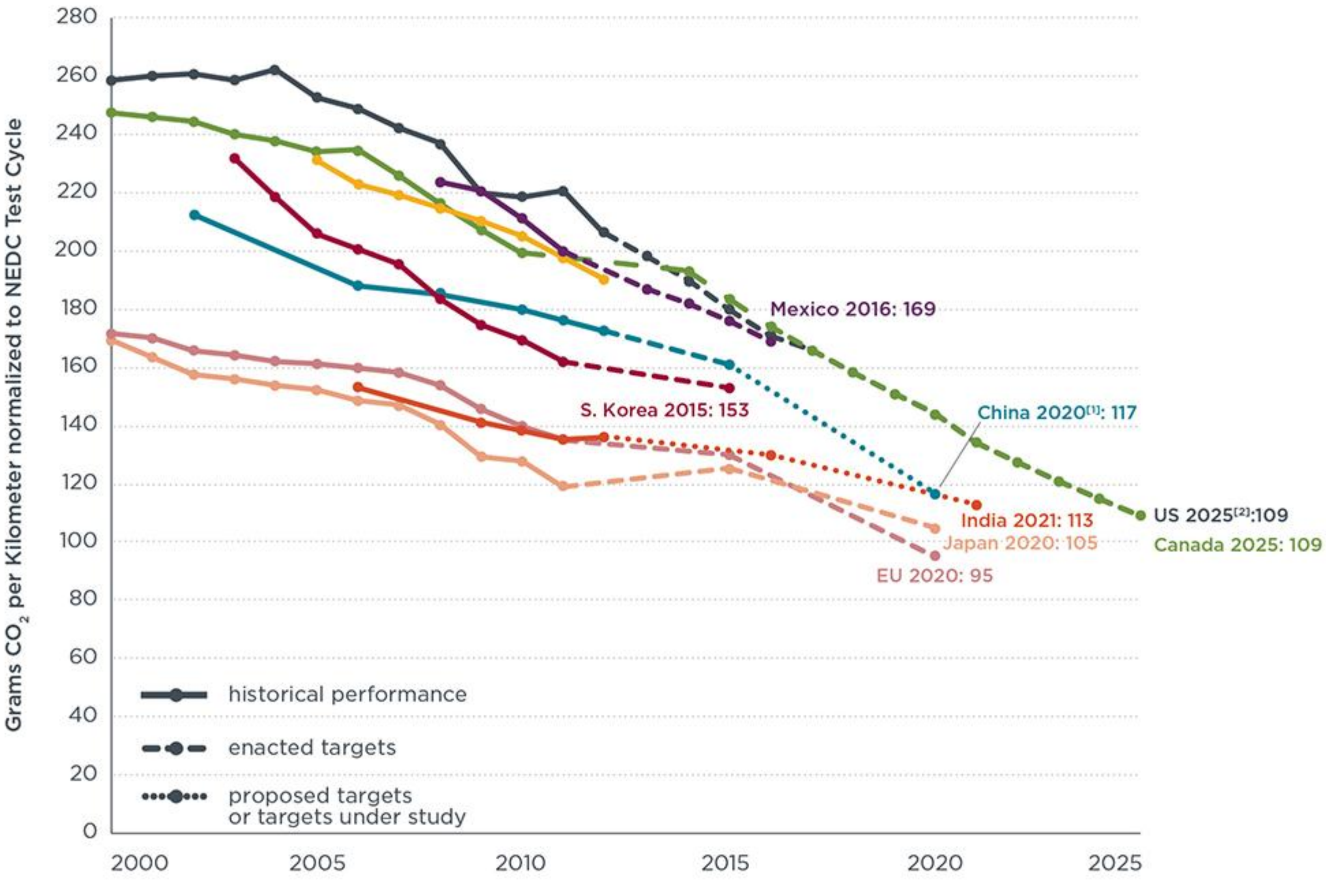
Light Vehicle Fleet CO_2 Targets



[1] China's target reflects gasoline vehicles only. The target may be higher after new energy vehicles are considered.
[2] US, Canada, and Mexico light-duty vehicles include light-commercial vehicles.
[3] Supporting data can be found at: http://www.theicct.org/info-tools/global-passenger-vehicle-standards

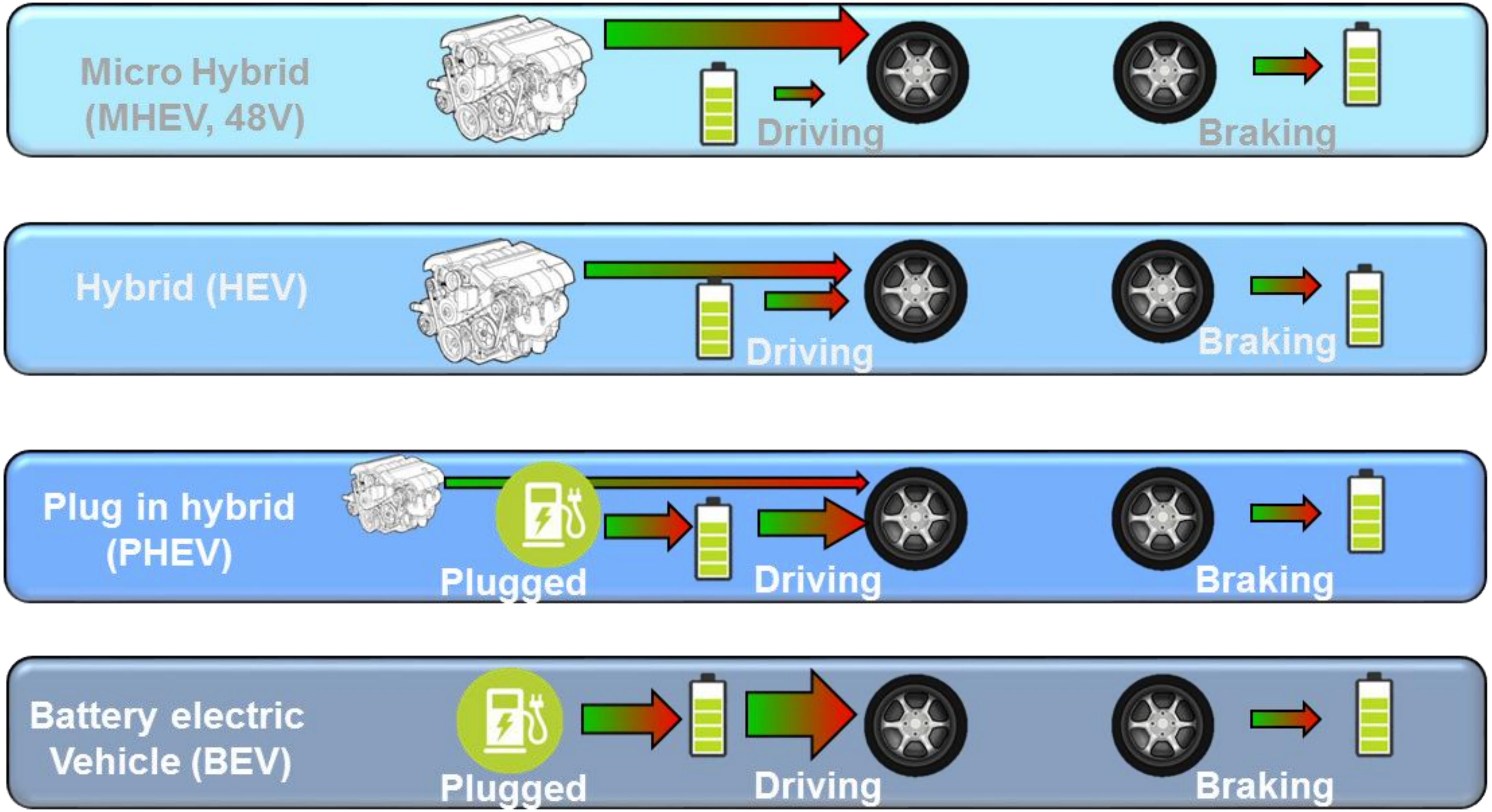
- **Global CO_2 emission targets are becoming more stringent**
- **A range of strategies are required to achieve the fleet average targets**
- **The electrified power train is the only credible zero emissions solution**

Why Batteries?

	Fuel cells	Fly wheels	Super-caps	Batteries	Downsized Engine
					
Energy density, *(Wh/kg)* *	0(800+)	70 – 130	1 – 85	30 – 1200	0(9K+)*
Power density *(W/Kg)***	650+	1K-100K	4K-100K	1K – 10K	800+
Temperature range	50^{0}C+	V.wide	-15-80^{0}C	-30-60^{0}C	V. wide
Technology maturity	★	★★½	★★	★★	★★★
Self discharge	★★	½	½	★★	★★★
Lifetime	★	★★★	★★★	★★	★★★
Cost	★	★★	★★	★★	★★★
Safety	★★	★★	★★	★★	★★
Zero emissions	★★★	½	½	★★★	

* Energy density of system energy source given, **Figures include research devices

Technology Introduction



Why Do We Need Different batteries?

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MHEV (Micro hybrid)

Charge from braking
-
Provide 48V power to auxiliaries
-
Limited Motor assist
-
High power required
-
V. Low energy storage
-
Only a small amount of the cells ability exploited

~11Kg
~15L
~0.5KWh
~>11kW peak
Nominal voltage: 42V
Peak current -230A

HEV

Charge from braking
-
Motor assist
-
Limited EV driving
-
High power required
-
Low energy storage
-
Only a small amount of the cells ability exploited

~50Kg
~50L
~1.5KWh
~>43kW peak
Nominal voltage: 260V
Peak current -180A

PHEV

Charge from the plug
-
Charge from braking
-
Motor assist
-
EV driving
-
High power required
-
High energy storage
-
Full cell capability exploited

~185Kg
~150L
~15KWh
~>130kW peak
Nominal Voltage:370V
Peak current -300A

BEV

Charge from the plug
-
Charge from braking
-
EV driving
-
High power required
-
High energy storage
-
Full cell capability exploited

~550Kg
~350L
~70KWh
~>290kW peak
Nominal Voltage:356V
Peak current -1000A

Low Cost, Low Impact — High Cost, High Impact

Improving Battery Performance

4x cost increase

2x cost increase

$66/kWh *
$LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$

0.570 kWh/kg
$LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$

$295/Kwh *
EV cell

0.150 kWh/kg
EV cell

$663/Kwh *
Total pack

0.080 Wh/kg (total)
(Nissan Leaf)

*Lowe, Tokuoka, Trigg & Gereffi;2010

70% Energy density reduction

50% Energy density reduction

Improving Battery Performance

Cell

X~100

Module

X12

Pack

22 kWh

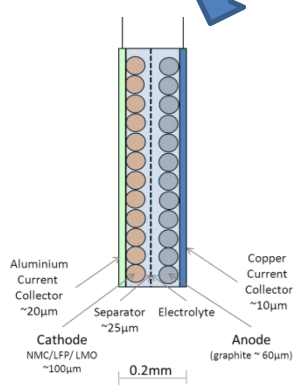
~300 kg

Aerodynamically optimised EV

Example:100 mile range

Active Material

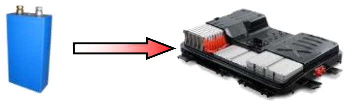
~48Kg



Cost/weight breakdown for large PHEV/Small EV	Cost*	Weight*
High Voltage wiring harness	4%	5%
High voltage isolation system	9%	4%
Heating system?	?%	?%
Mechanical Harness	4%	7%
Packaging	5%	15%
Cooling system	2%	4%
Low voltage wiring harness	1%	2%
Electronic control modules	9%	3%
Cell	49%	60%
Fixed costs, Warranty, Profit £	18%	-

*Cost and Weight Breakdown adapted from 'Cost and Performance of EV batteries' report for The committee on Climate Change 2012

Battery Design Choices



Chemistry	Cell type	Cooling system	BMS	Module	Packaging
LFP	Prismatic	Passive	Centralised	Cassettes	Metal
NMC	Cylindrical	Forced air	Master/Slave	Banding	Composite
LMNO-(spinel)	Pouch	Liquid	Distributed	Enclosed	Body integrated
Supplier choice, voltage Window, lifetime, power @ SOC	Supplier choice, Thermal properties, Power rating,	Drive cycle, Power requirement, Market, Battery size,	Cost, Flexibility Reliability, Safety,	Cost, serviceability Reliability, Safety, weight	Cost, Vehicle platform, Reliability, Safety, weight

How does the Micro affect the Macro?

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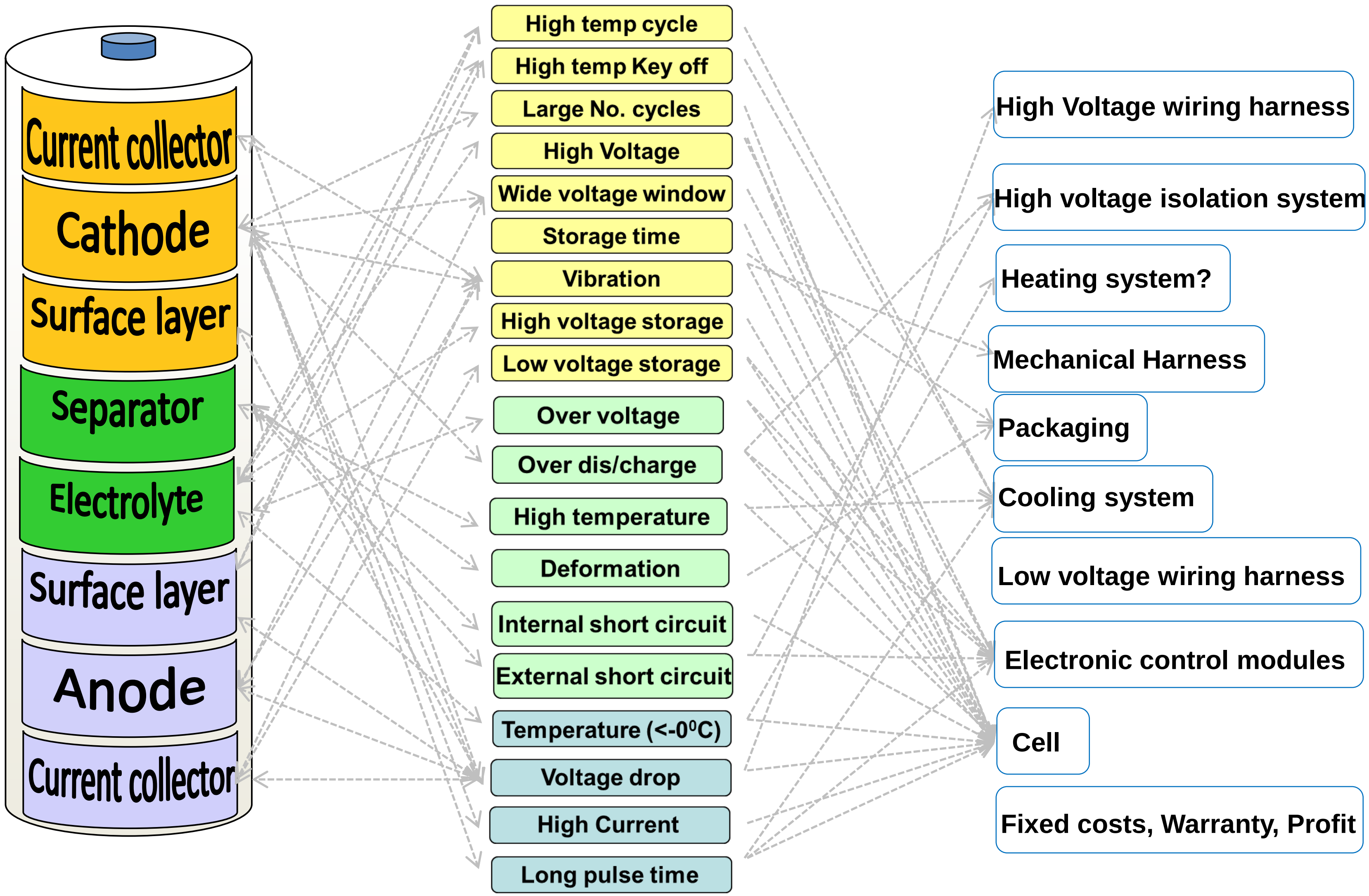
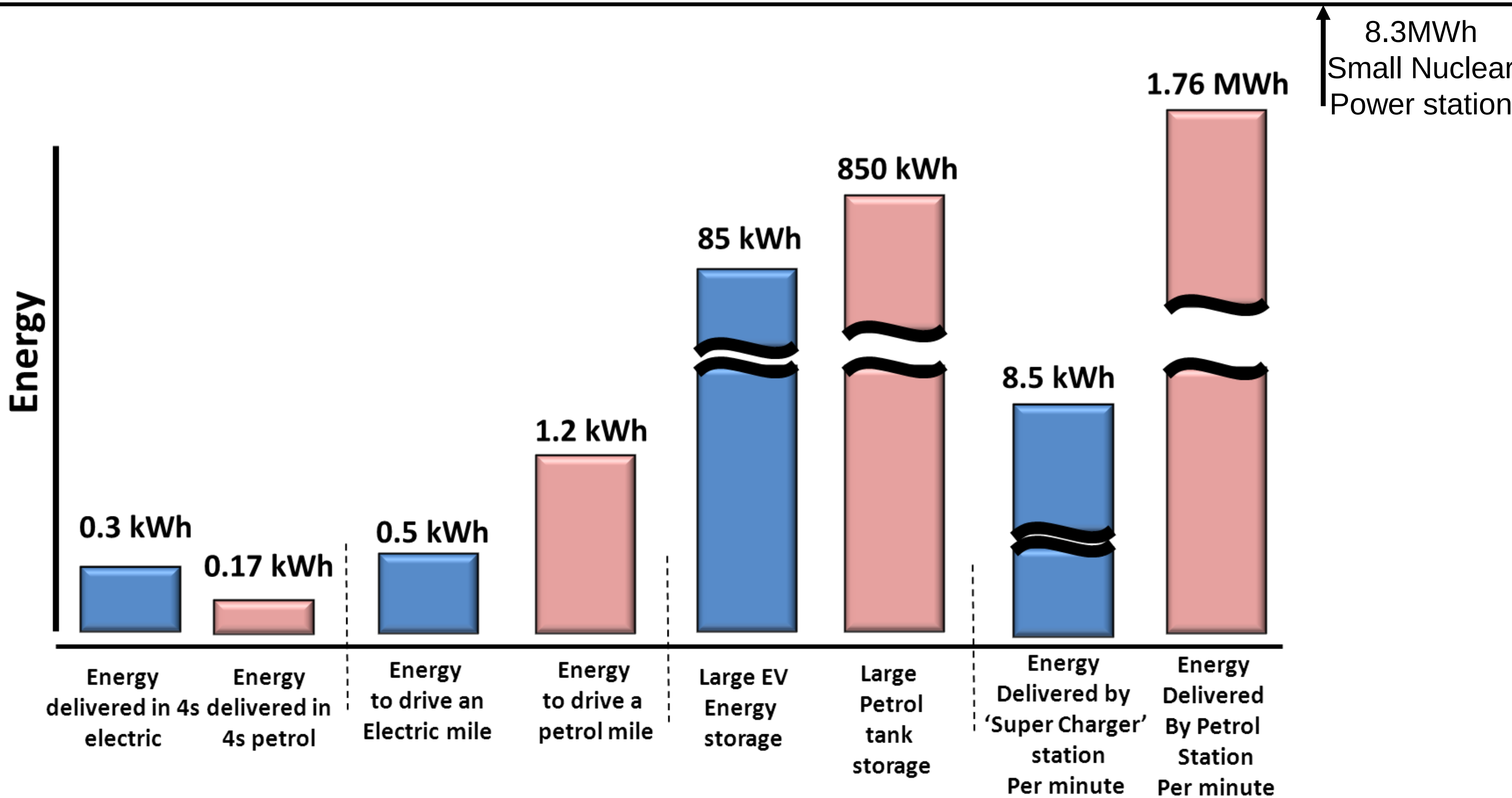
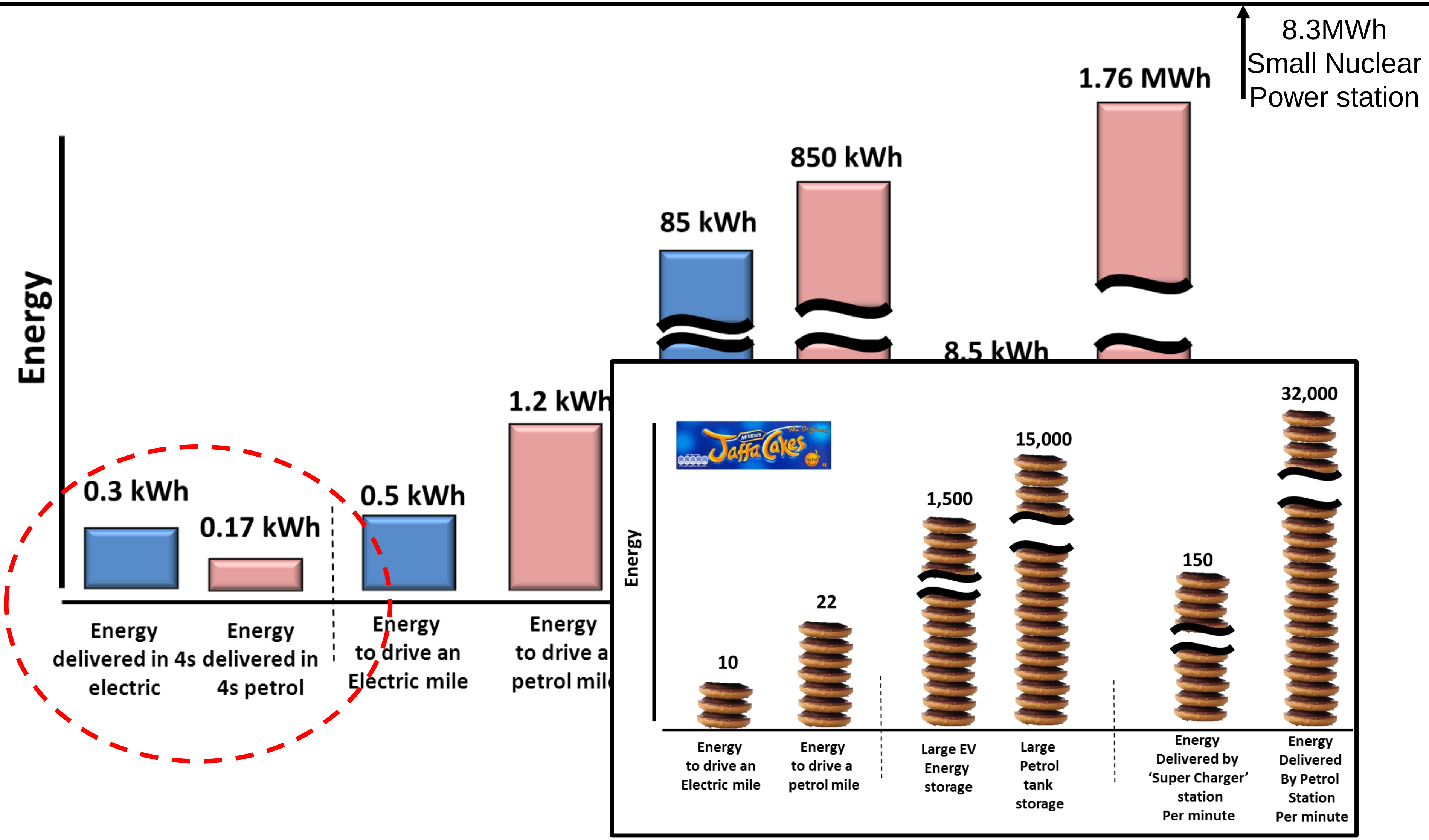
Cell Material | **Failure Trigger** | **Pack containment**



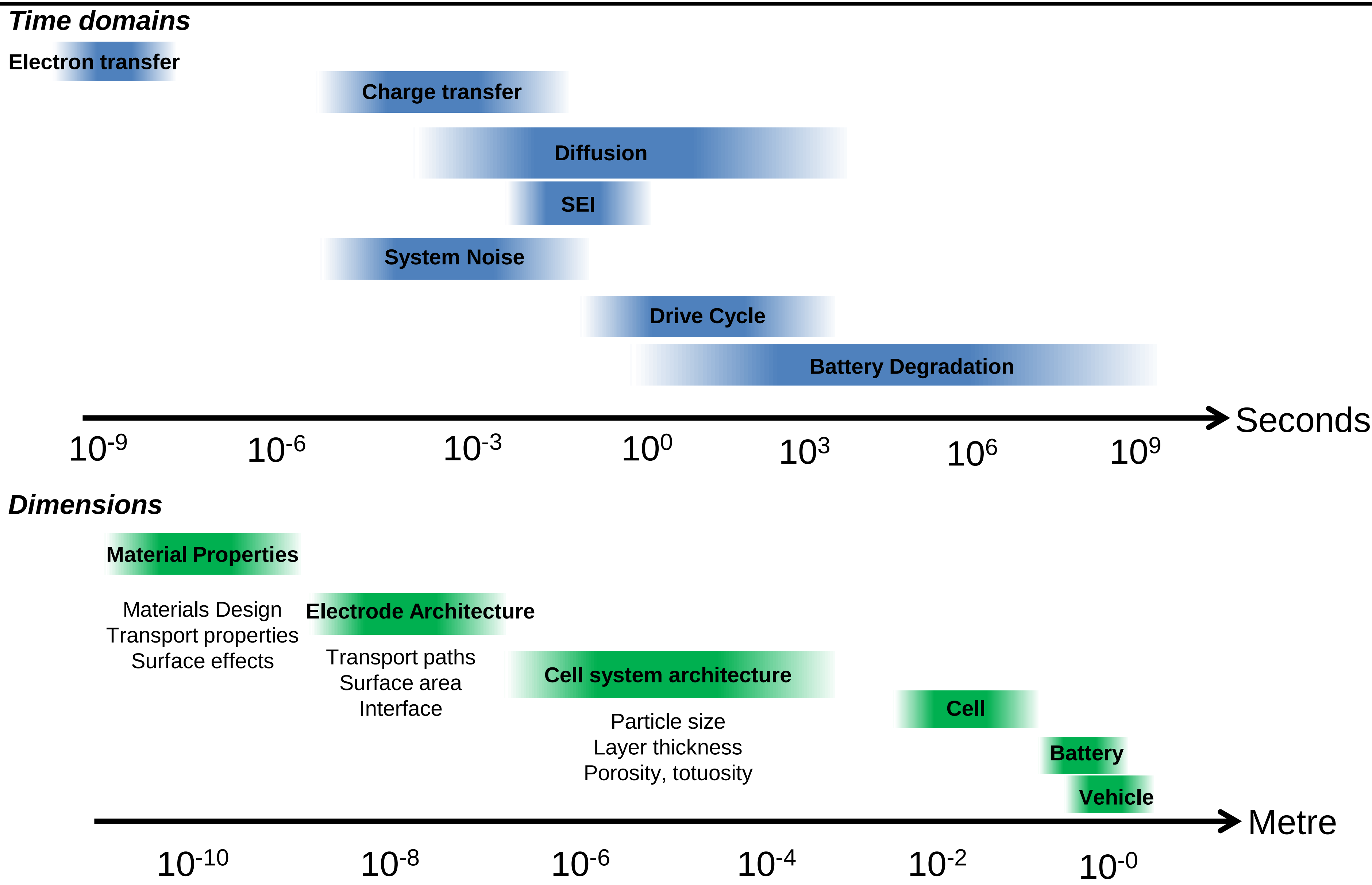
Key Battery metrics



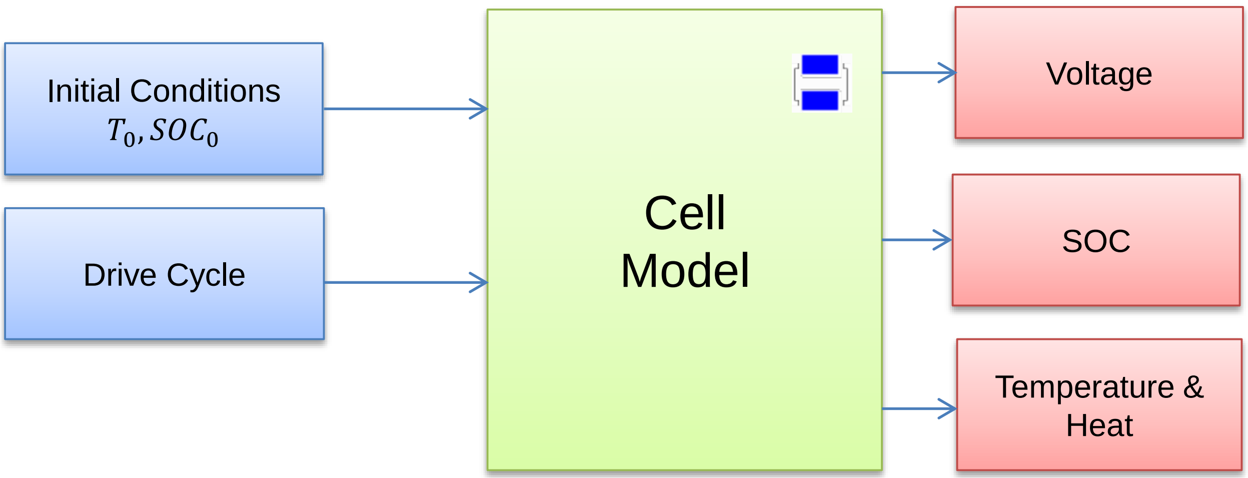
Key Battery metrics



Vehicle System Challenges



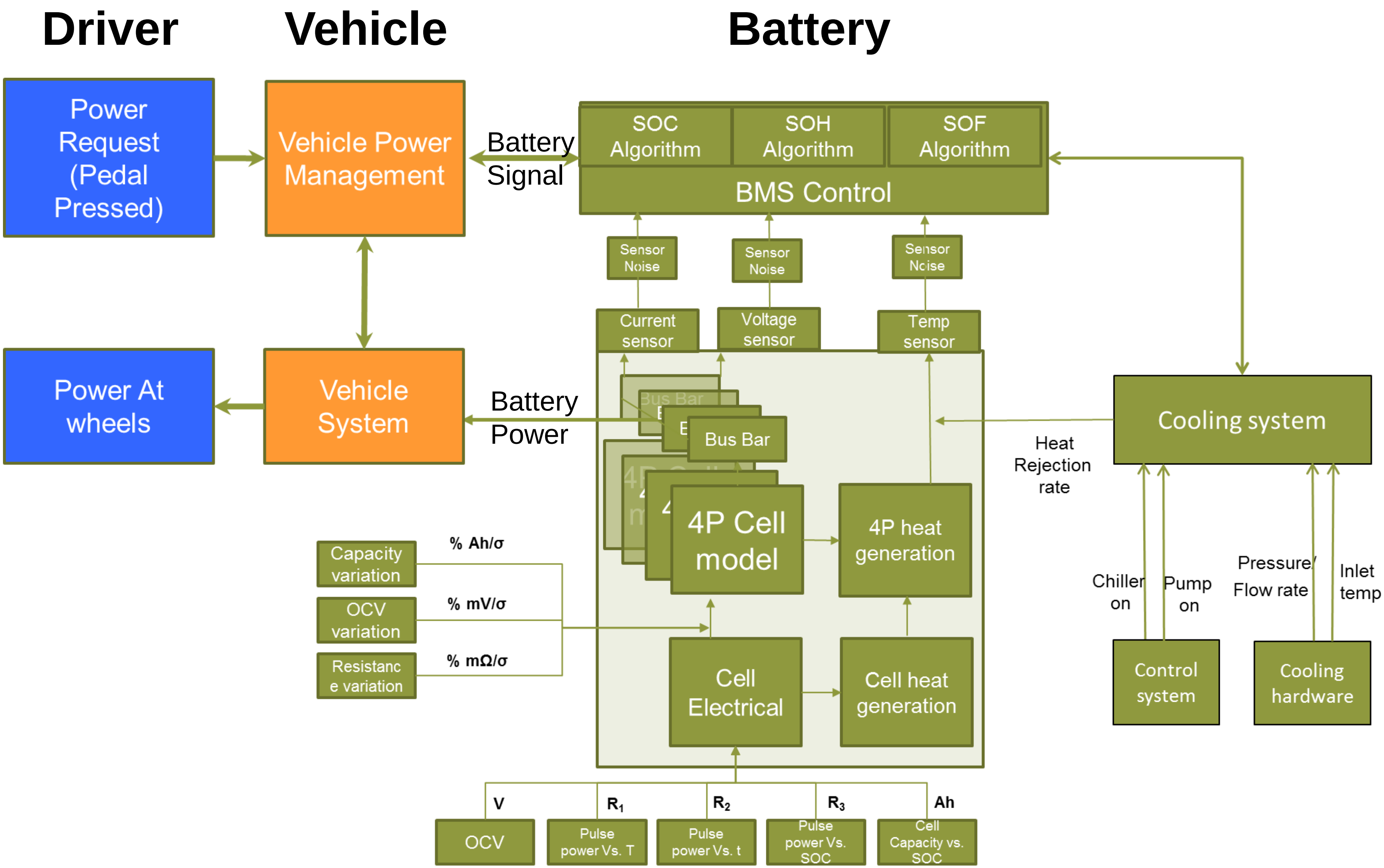
Electro-Thermal Model Requirements



Requirements

- Spatially resolved(thermally)
- Model outputs correct to less than 2% error
- Valid in temperature range $-40 \leq T \leq 60$
- Cells in a pack are uniquely parameterisable
- Paramatised within 2-3 months
- Runs close to real time

System Model Context



Electrical Modelling Approaches

Basic

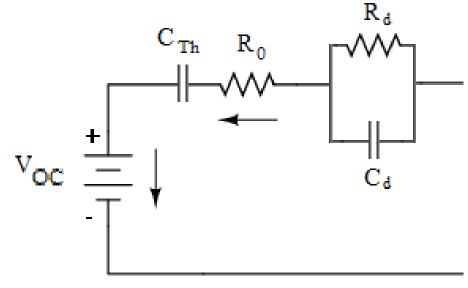
$$P=I.V_{ocv}+I^2.R$$

Analogy

Characterisation time
1 Day-1week

Run time: <real time

Equivalent Circuit

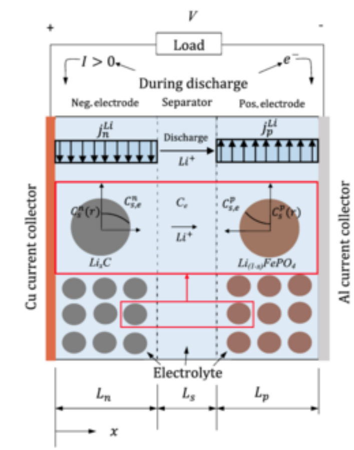


Phenomenological

Characterisation time
1 week-1 month

Run time: <real time

Electrochemical



$$j^{Li} = a_s i_o \left\{ \exp\left[\frac{\alpha_a F}{RT}\eta\right] - \exp\left[-\frac{\alpha_c F}{RT}\eta\right] \right\}$$

$$i_0 = k(c_e)^{\alpha_a}(c_{s,\max} - c_{s,e})^{\alpha_a}(c_{s,e})^{\alpha_c}$$

$$\eta = (\phi_s - \phi_e) - U$$

Mechanistic

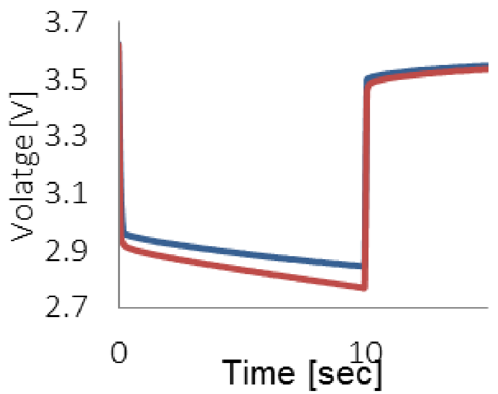
Characterisation time
6 months -1 year

Run time: >real time

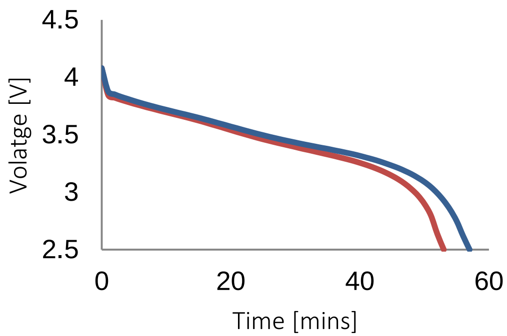
Tanvir R. Tanim, Christopher D. Rahn (2015 *Journal of Power Sources*, Volume 294, Pages 239-247

Characterisation requirements

Basic



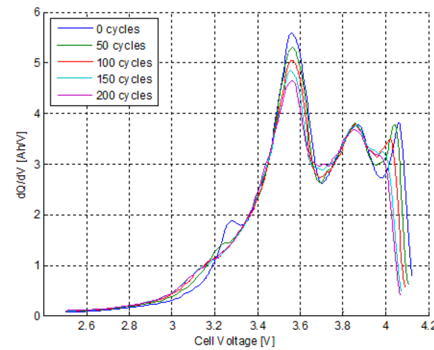
Pulse Power



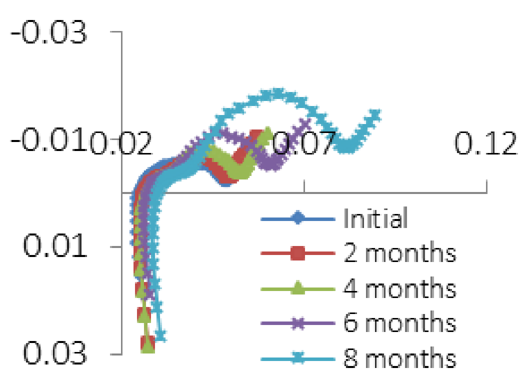
Constant Discharge

Equivalent Circuit

[5]



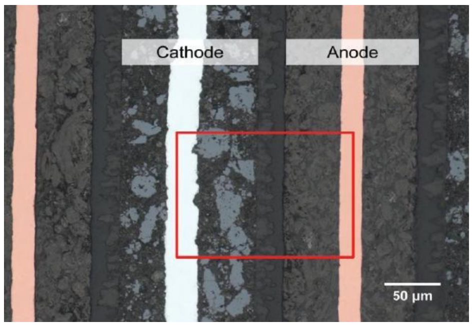
Incremental Capacity



EIS Tests

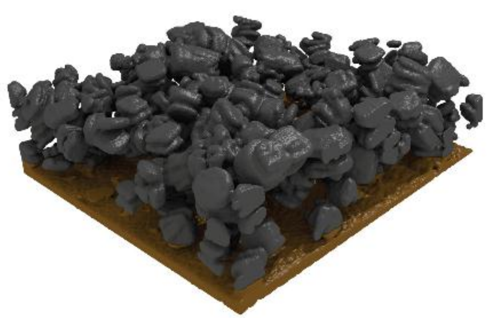
Electrochemical

[3]



SEM imaging

[4]

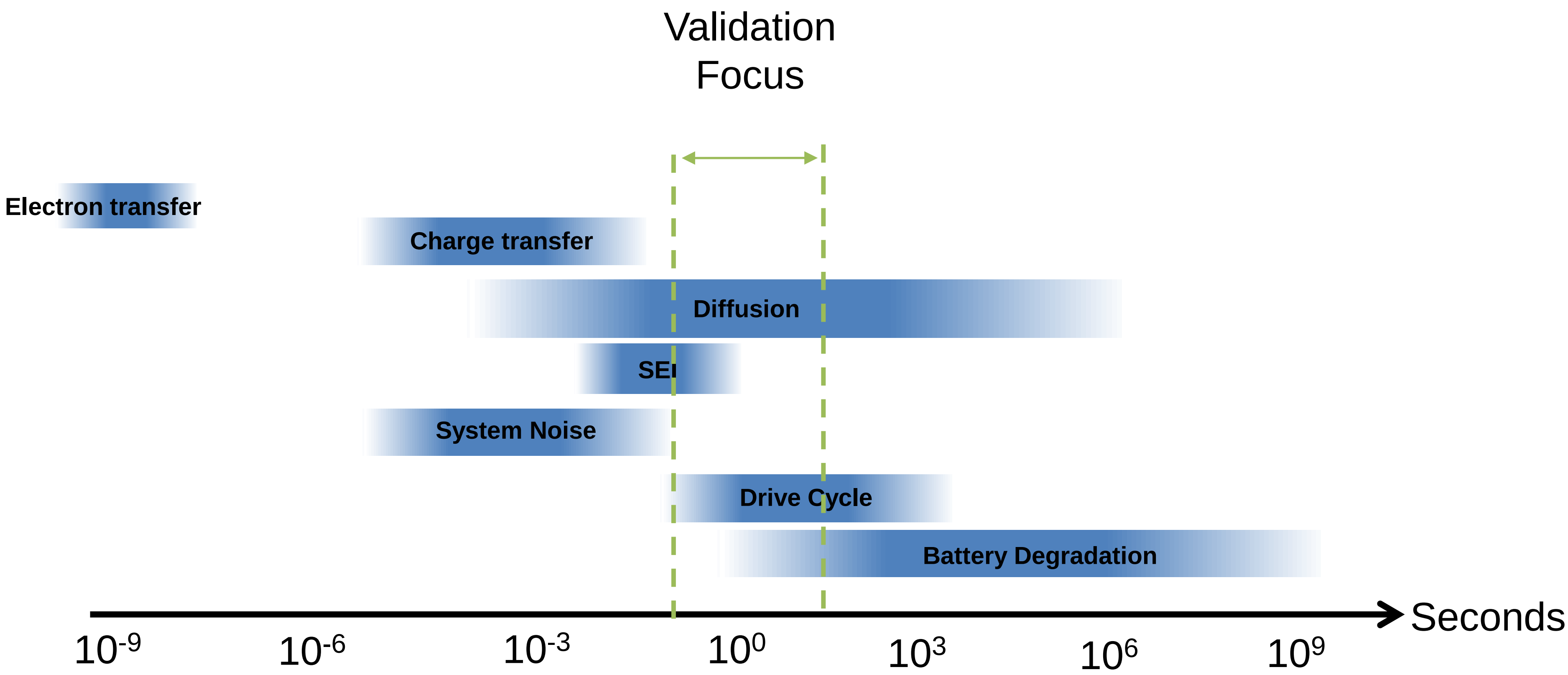


Tomography

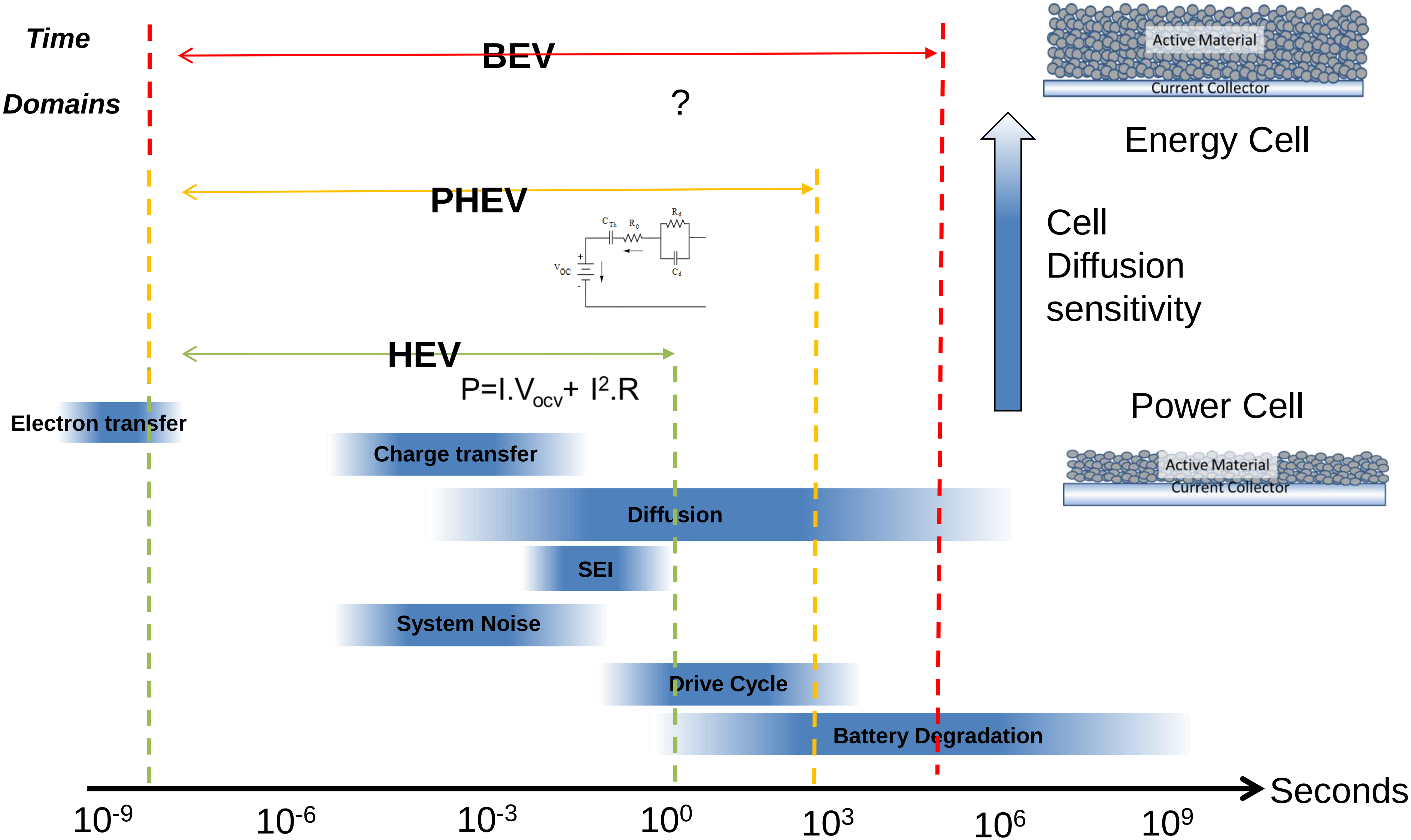
[3] Y. Li et. al., "Mesoporous Co_3O_4 nanowire arrays for lithium ion batteries with high capacity and rate capability." *Nano Letters* 8.1 (2008): 265-270.
[4] M. Ebner, Laboratory for Nanoelectronics, ETH Zurich
[5] C. Pastor-Fernández , K. Uddin, J. Marco, WMG, University of Warwick

A Problem of Validation

Time Domains



The Changing nature of modelling requirements



What next?

- Vehicle system modelling has to become more sophisticated
- Better understanding of battery fundamental mechanisms is crucial
- Increasing focus on ground up modelling of battery systems

But….

- The Challenges is not just in building the model
- Rapid characterisation & run speed are crucial for wide stream uptake

Thankyou