

# trainThermoNetNew

March 16, 2022

```
[219]: import numpy as np
import torch
from torch.utils.data import DataLoader
from torch.optim import RMSprop, SGD
from torch.optim.lr_scheduler import ExponentialLR
from torch.nn import MSELoss
import matplotlib.pyplot as plt

from thermonet.net import ThermoNetNew
from thermonet.dataset import ThermoDatasetNew
from utils.plot import PlotHandler

[213]: def epoch(net, dataloader, loss_func, optimizer, scheduler):
    epoch_losses = np.zeros([len(dataloader), ])

    for i, d in enumerate(dataloader):
        inp = d[:, [0, -2, -1]]
        targets = d[:, [1, 2, 3, 4]]

        # Forward pass
        predictions = net(inp.float())

        # Get the loss
        loss = loss_func(predictions, targets.float())

        # Backward pass
        net.zero_grad()
        loss.backward()
        optimizer.step()
        epoch_losses[i] = loss
    scheduler.step()

    mean_epoch_loss = epoch_losses.mean(axis=0)
    #print('Mean epoch loss: ', mean_epoch_loss)
    return mean_epoch_loss

def train(net, dataloader, optimizer, scheduler, loss_func, nr_epochs=500):
    losses = []
```

```

best_loss = epoch(net, dataloader, loss_func, optimizer, scheduler)
best_net = net

ph = PlotHandler()

for i in range(nr_epochs):
    #print('-----\nEpoch %i:\n' % i)
    loss = epoch(net, dataloader, loss_func, optimizer, scheduler)
    losses.append(loss)

    if loss < best_loss:
        best_net = net

    if i % 10 == 0:
        print(i, ': ', loss)
        print('lr: ', scheduler.get_last_lr())
        last_losses = np.array(losses[-50:])
        last_losses_std, last_losses_mean = last_losses.std(), last_losses.
↪mean()

        last_loss_diffs = np.diff(last_losses)
        print(np.mean(last_loss_diffs))
        print(last_losses_std/np.mean(last_loss_diffs), last_losses_std, ↪
↪last_losses_mean)
        print()

        if i % 250 == 0:
            ph.properties_temp_modified_new(best_net, ['C'], 'LIQUID', ↪
↪start_temp=200, end_temp=2000)
            plt.plot(losses)

    return losses, net

```

```

[214]: # Hyperparameters
nr_epochs = 25000
lr = 0.005 # 0.000025
batch_size = 256
hidden_size = 128
hidden_layers = 8

```

```

[215]: # Network
net = ThermoNetNew(hidden_size_linear=hidden_size, hidden_layers=hidden_layers)

# Optimizer
optimizer = RMSprop(net.parameters(), lr=lr)
scheduler = ExponentialLR(optimizer, gamma=0.995)

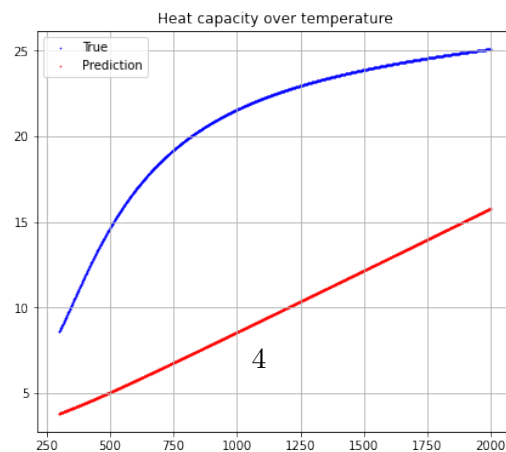
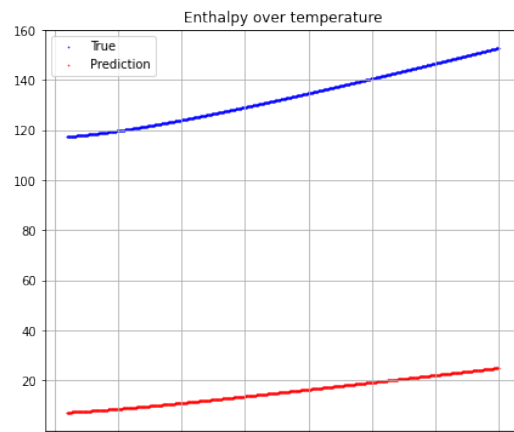
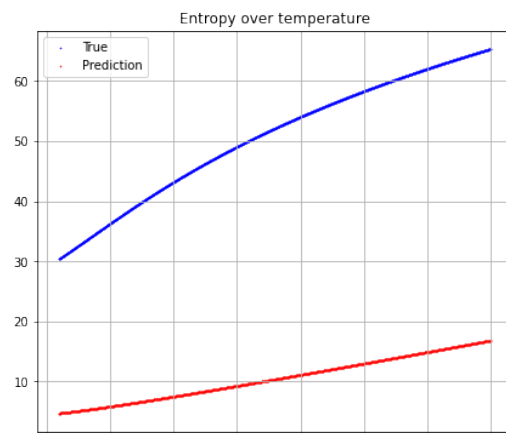
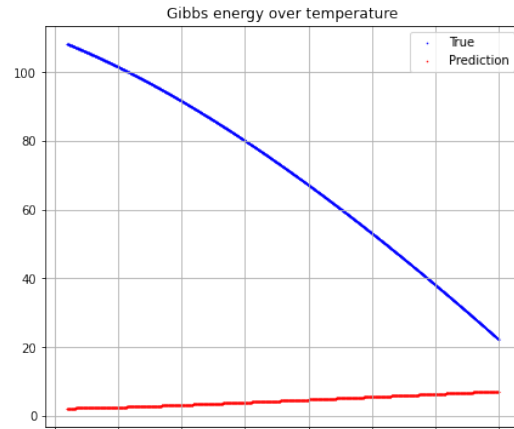
```

```
# Loss function
loss_func = MSELoss()
```

```
[216]: # Dataset
start_temp, end_temp = 200, 2000
step = 10
dataset = ThermoDatasetNew(['C'], start_temp=start_temp, end_temp=end_temp,
    ↪step=step)
dataloader = DataLoader(dataset, batch_size=batch_size, shuffle=True)
```

```
[217]: losses, best_net = train(net, dataloader, optimizer=optimizer,
    ↪scheduler=scheduler, loss_func=loss_func, nr_epochs=nr_epochs)
```

```
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lr: [0.0049501250000000005]
nan
nan 0.0 1180040.7841796875
```



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 lr: [0.004477934953669392]  
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50 : 1363.38525390625  
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445062.8724023615 67.07963912115072 1355.6441552734375

210 : 1336.3407592773438

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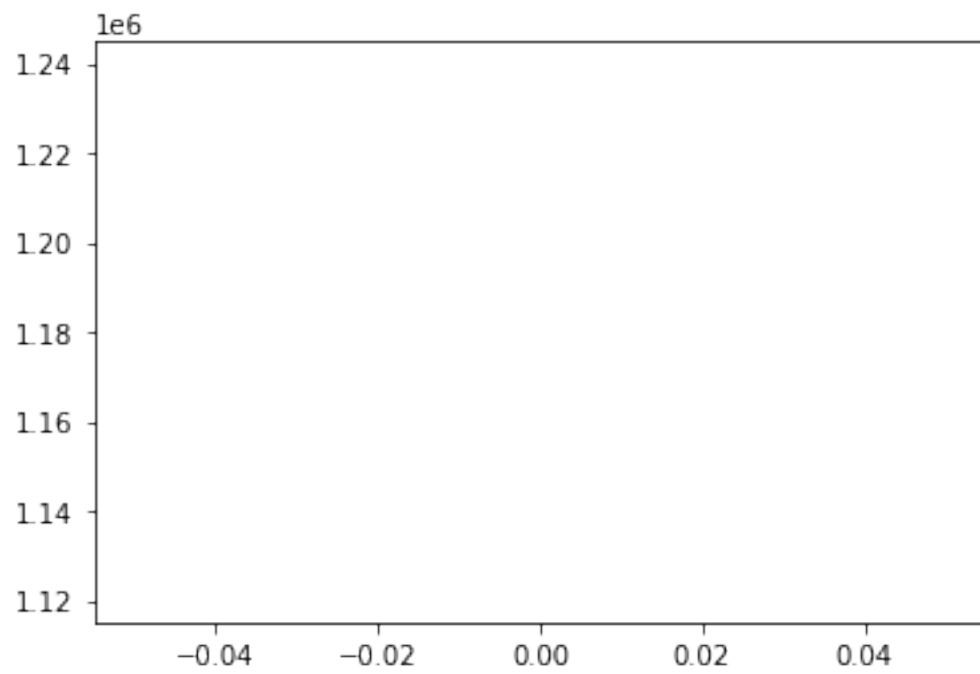
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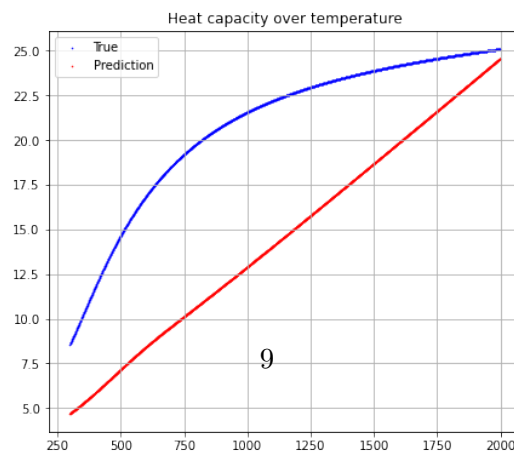
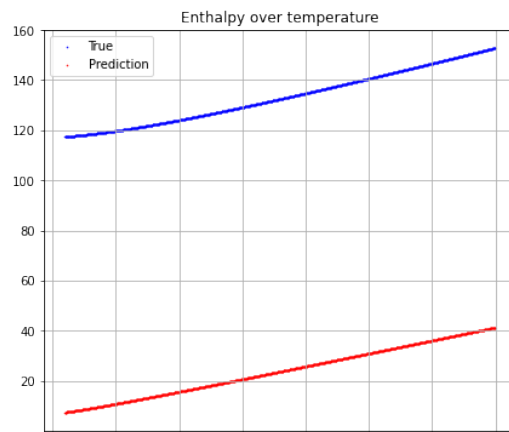
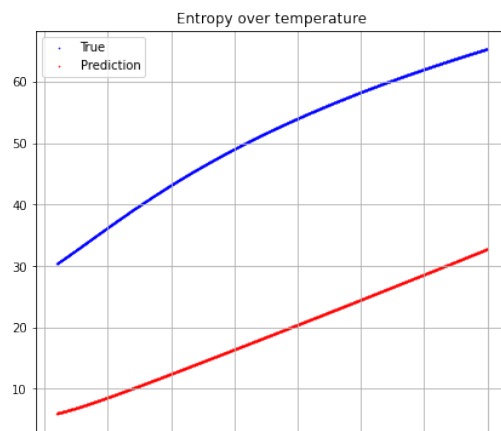
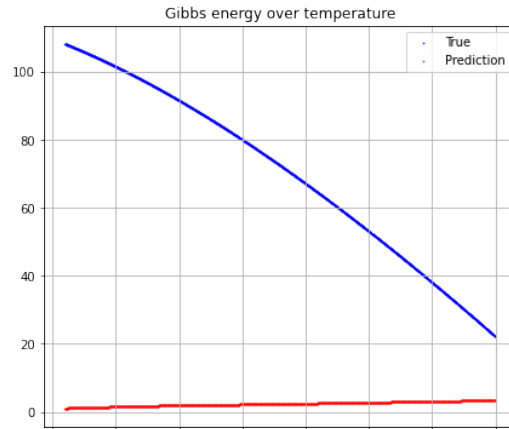
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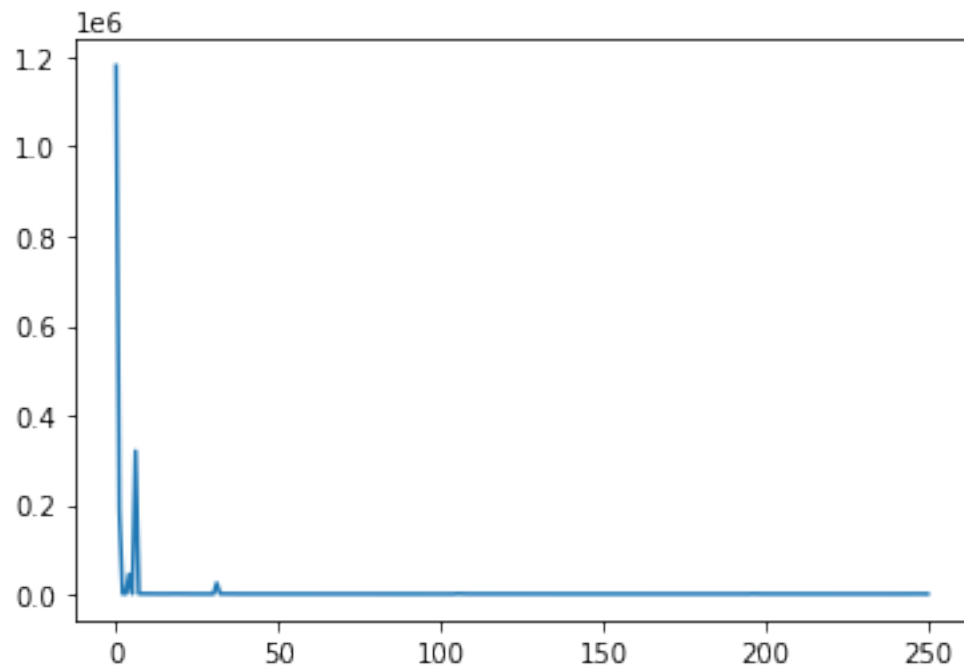
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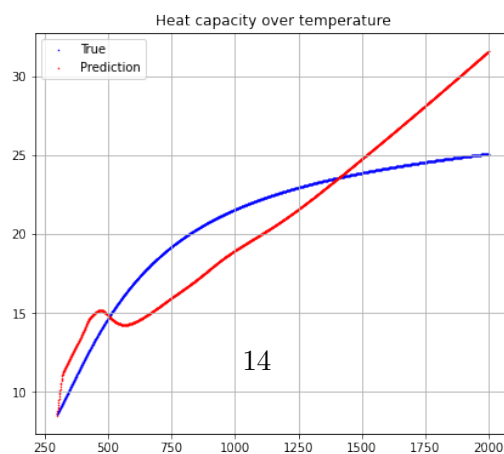
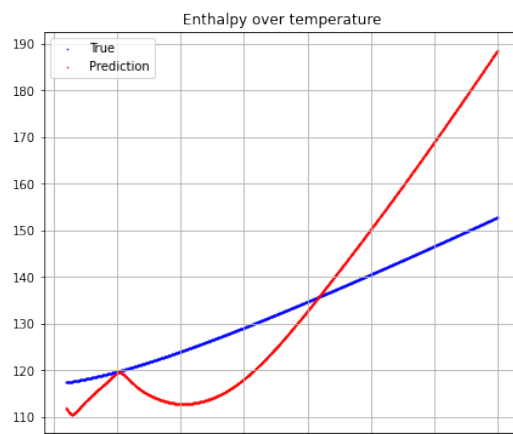
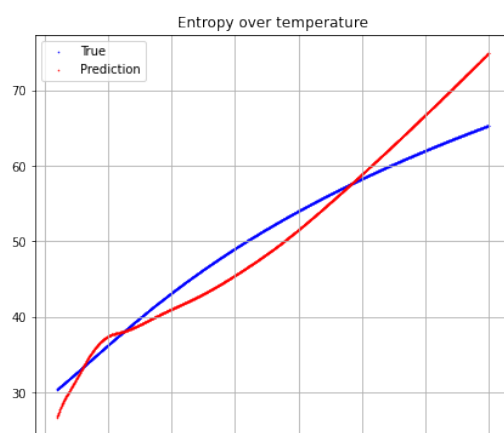
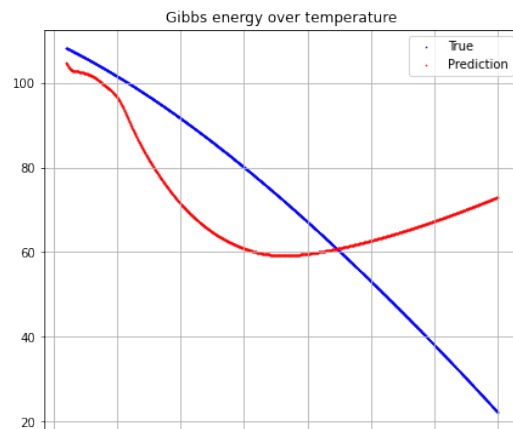
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500 : 216.24219512939453  
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670 : 17.694847106933594  
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 lr: [0.00015579082615644384]  
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700 : 8.330331802368164

lr: [0.00014817423299102564]

-0.29721768048344827

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710 : 13.980978965759277

lr: [0.00014093001407176005]

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720 : 11.069224834442139

lr: [0.0001340399640703348]

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730 : 11.72657299041748

lr: [0.0001274867677145635]

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-22.587290421717857 6.490309592839561 15.749345560073852

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lr: [0.00012125395627365804]

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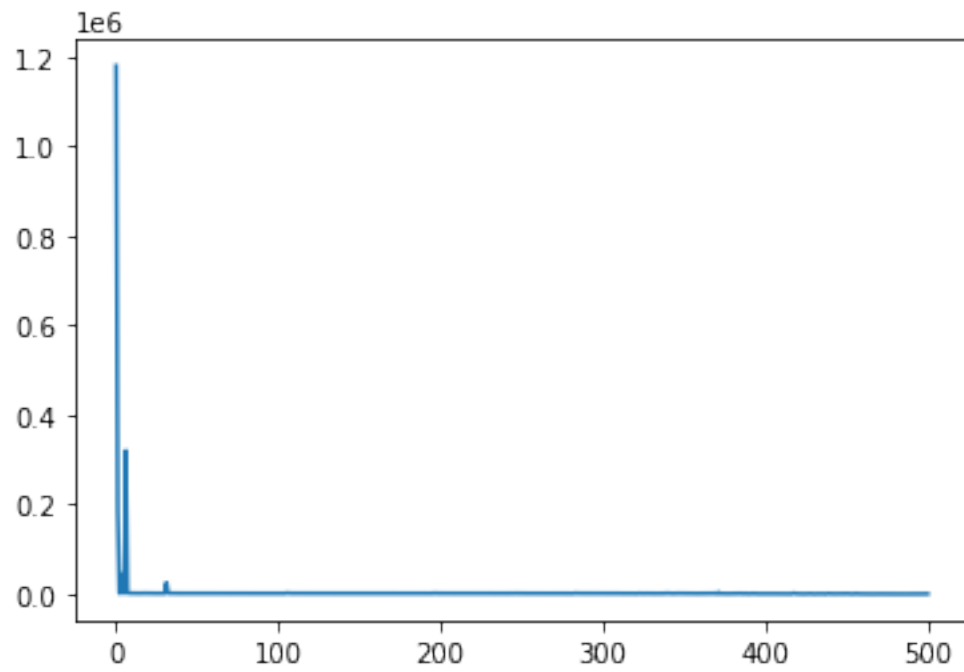
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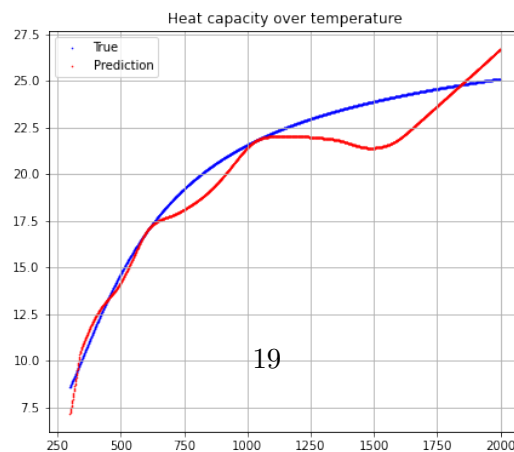
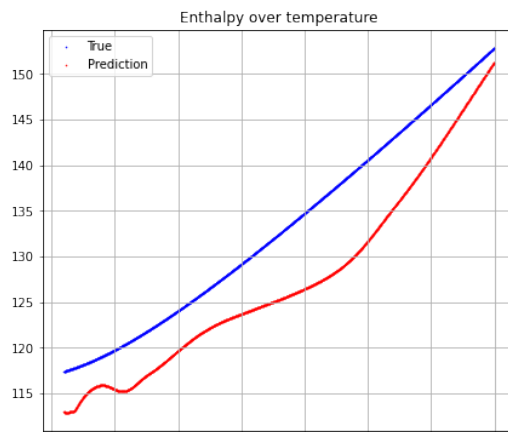
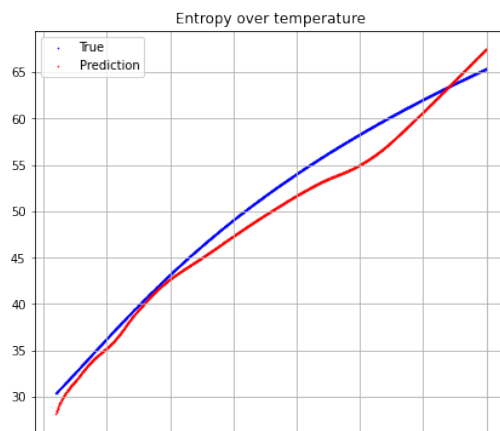
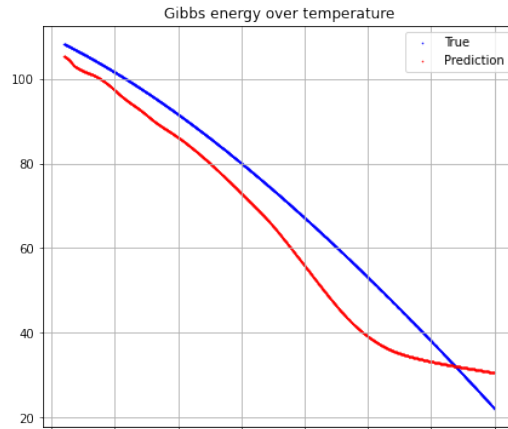
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lr: [0.0001153258661709299]

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760 : 8.90294885635376  
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770 : 9.37854290008545  
 lr: [0.00010432498718497115]  
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780 : 6.524272680282593  
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790 : 5.167064666748047  
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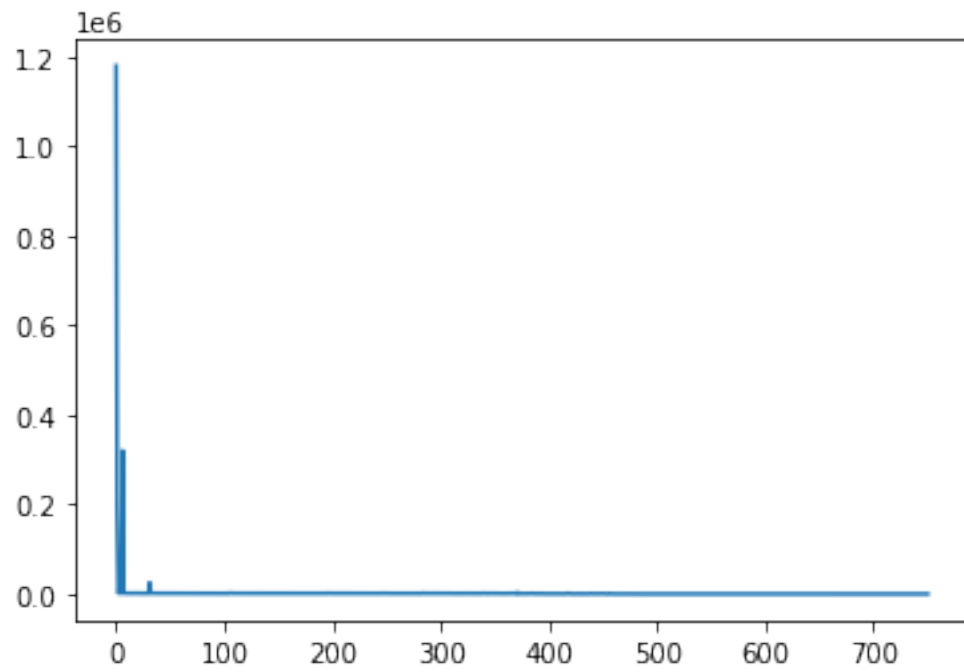
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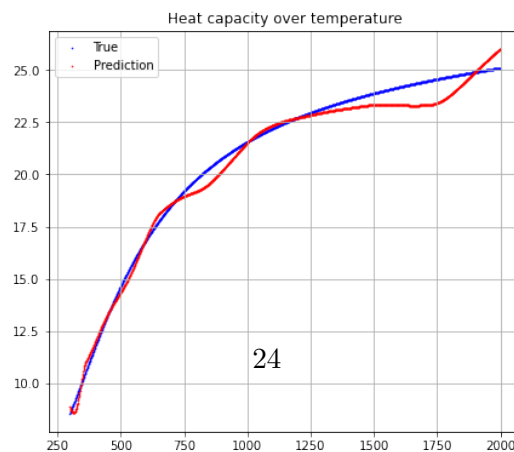
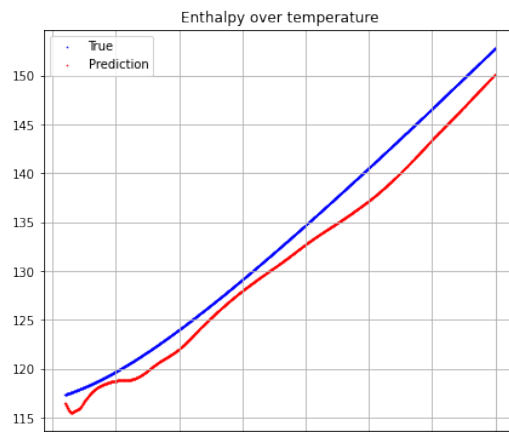
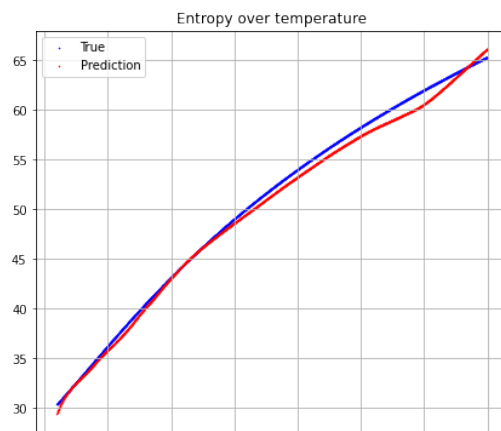
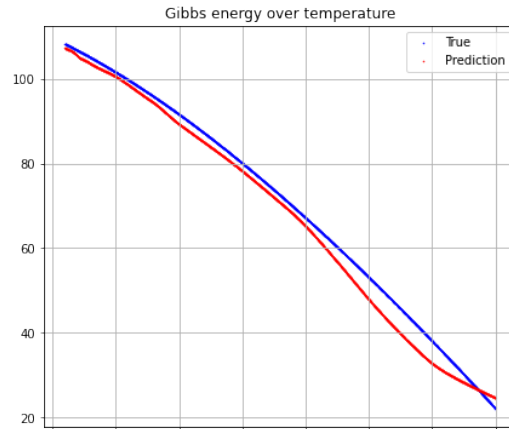
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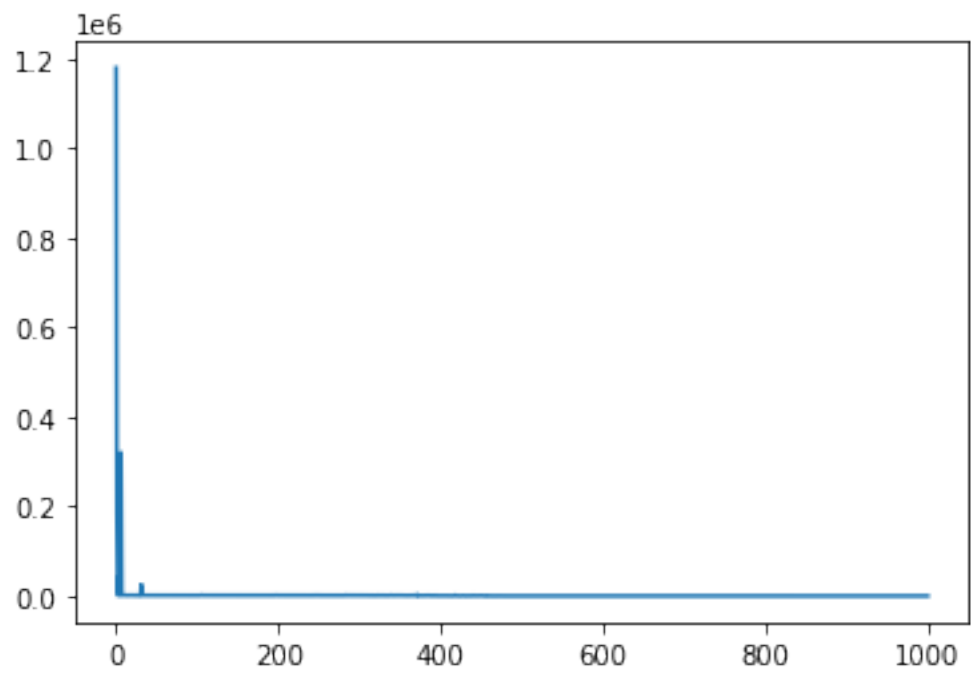
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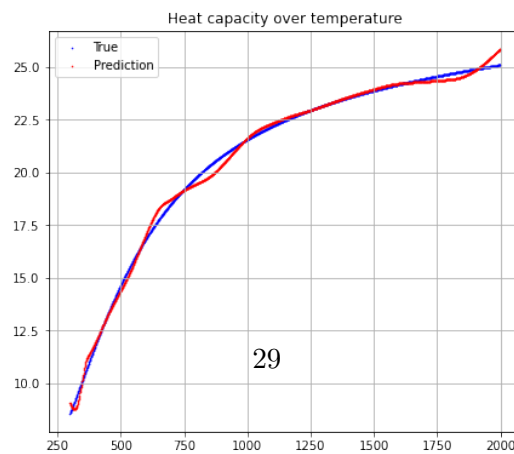
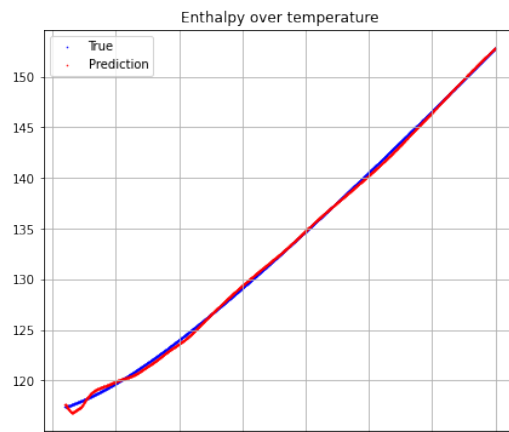
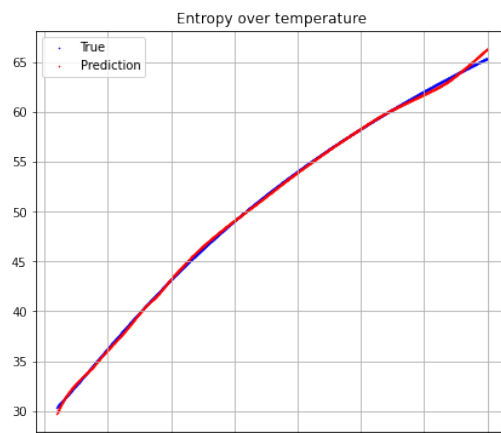
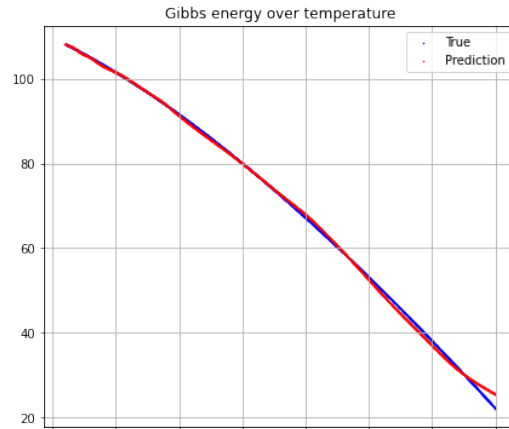
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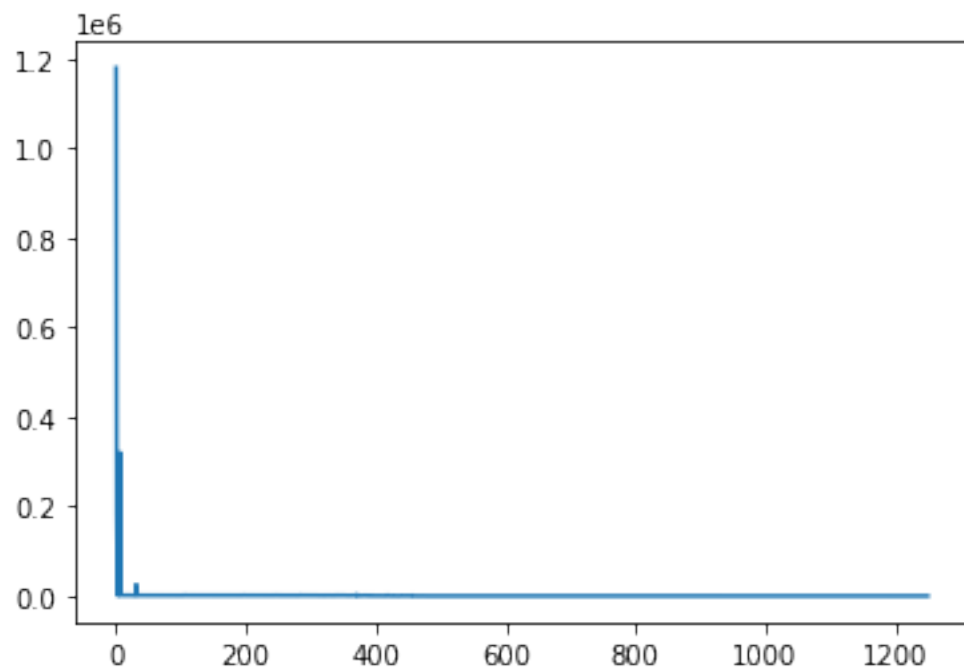
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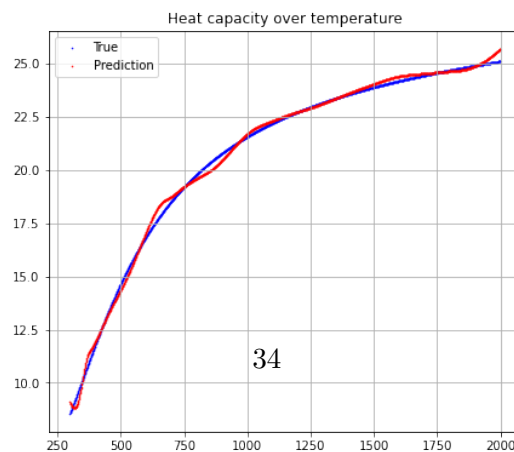
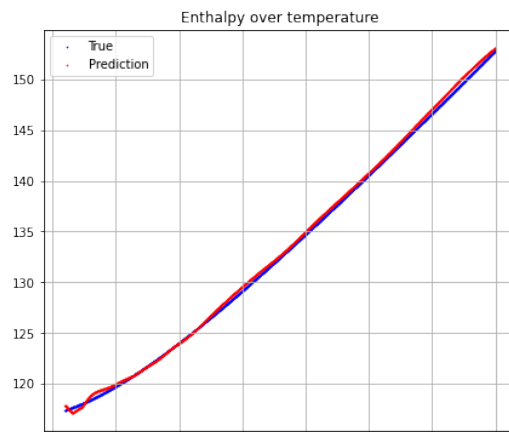
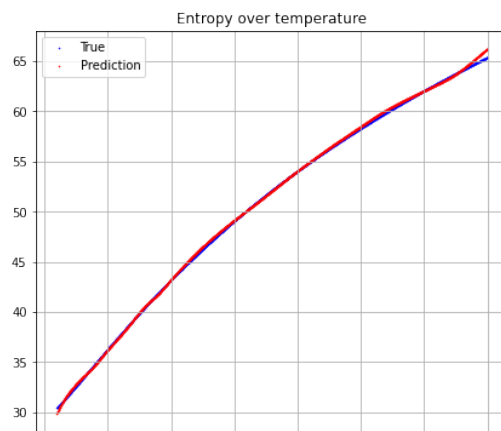
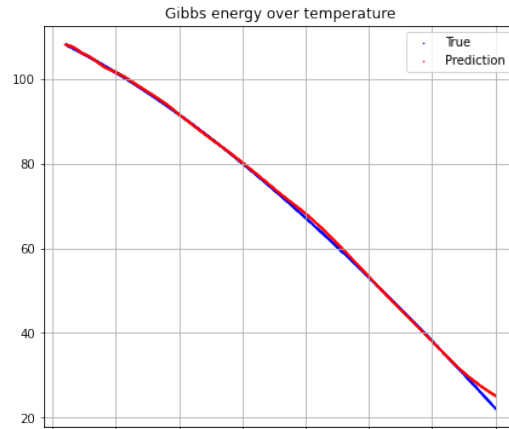
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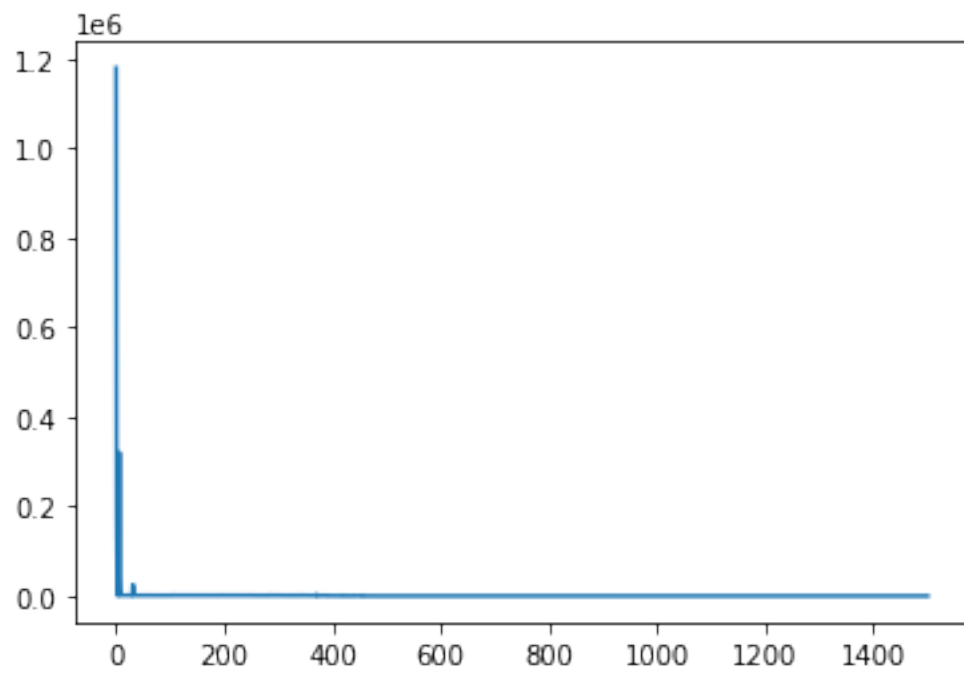
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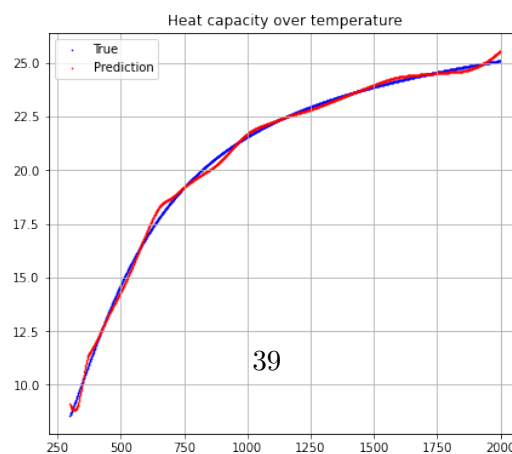
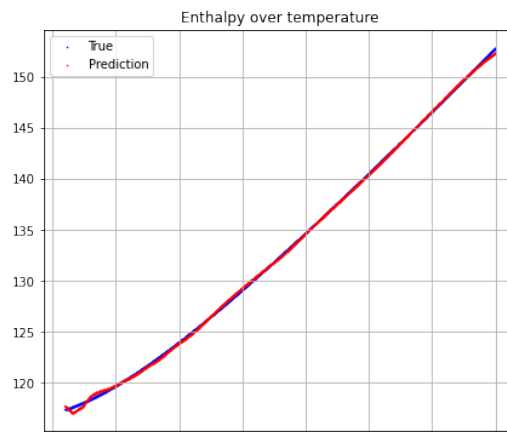
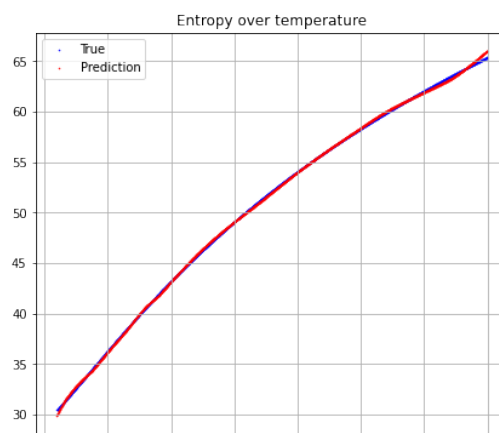
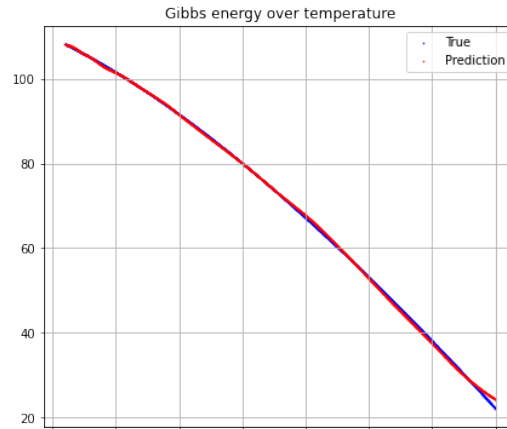
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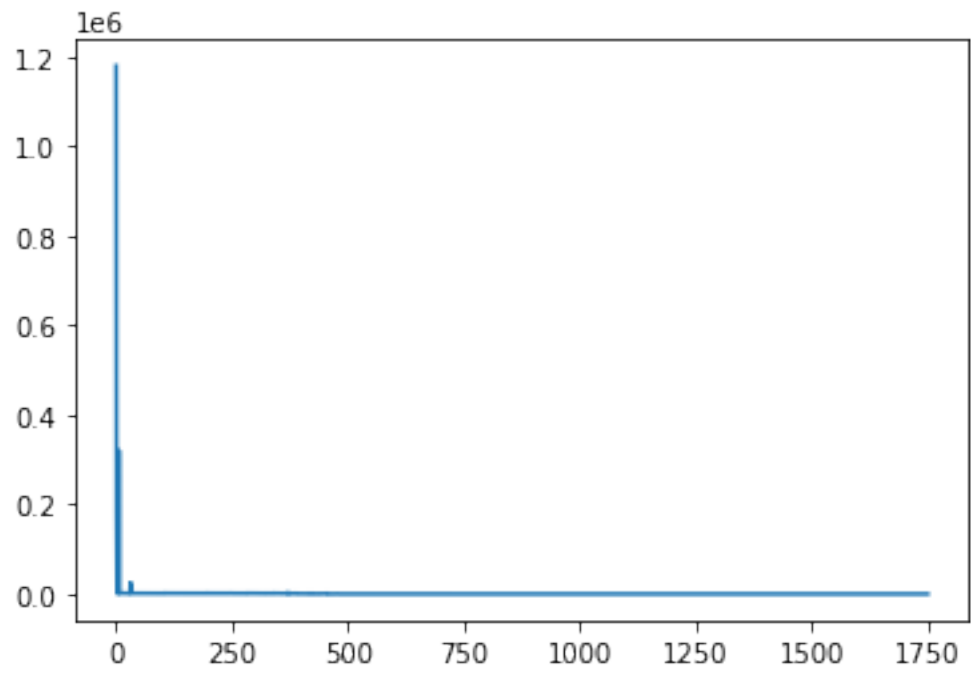
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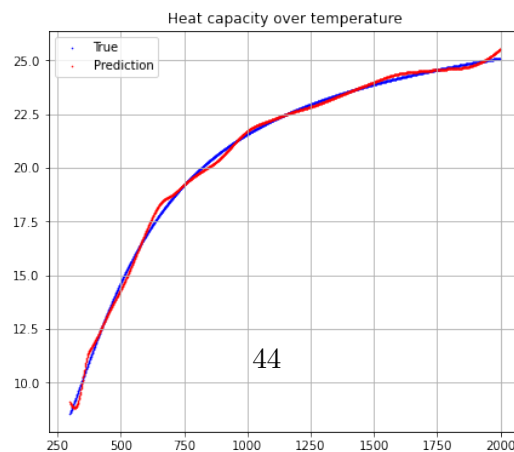
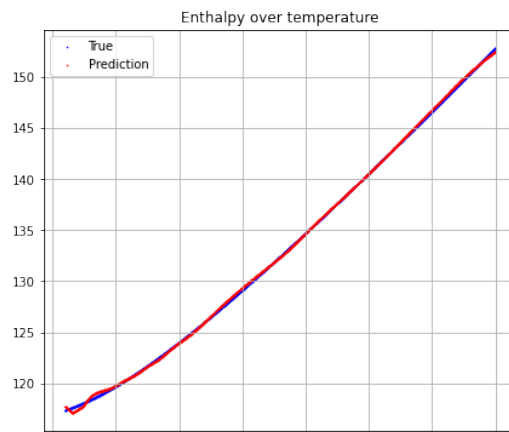
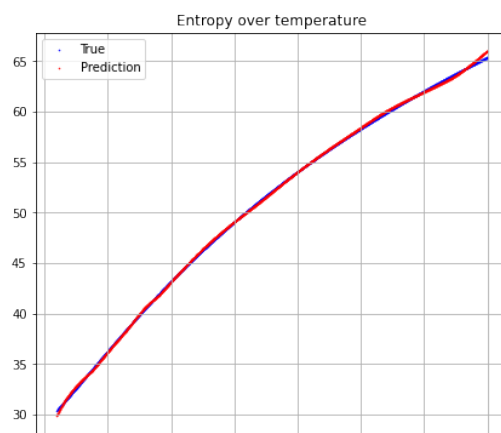
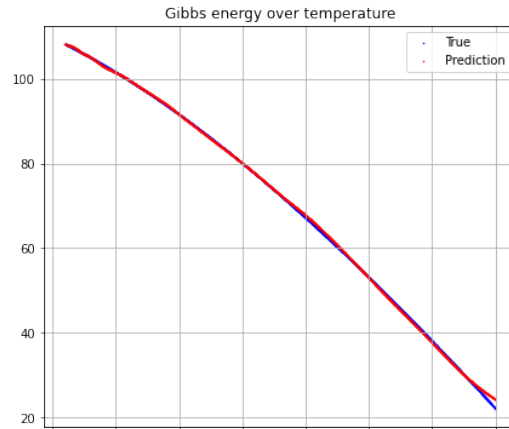
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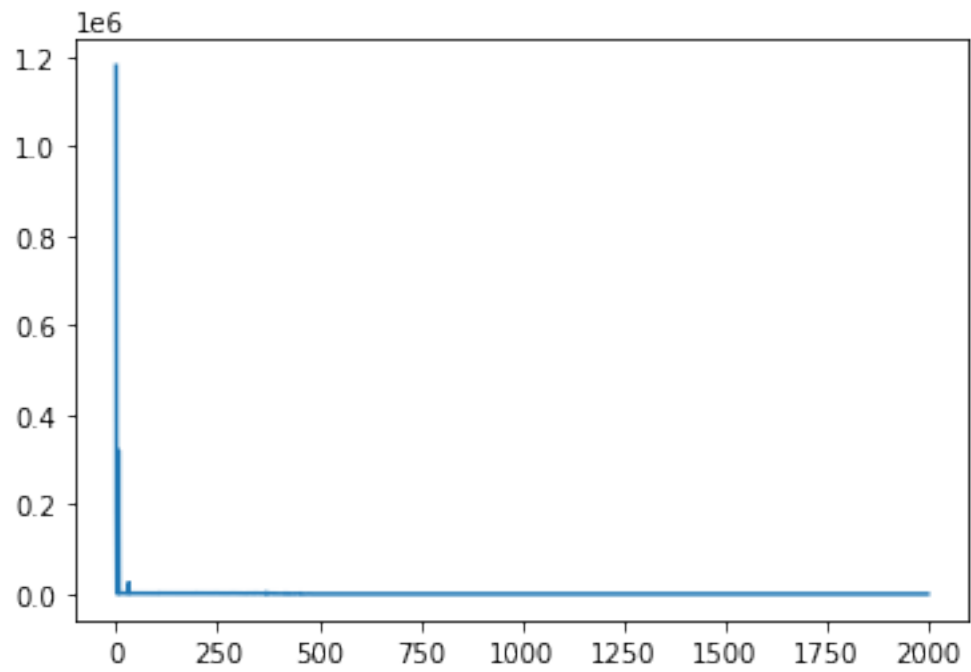
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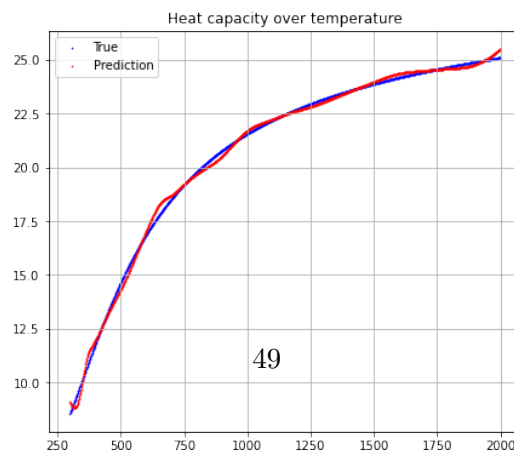
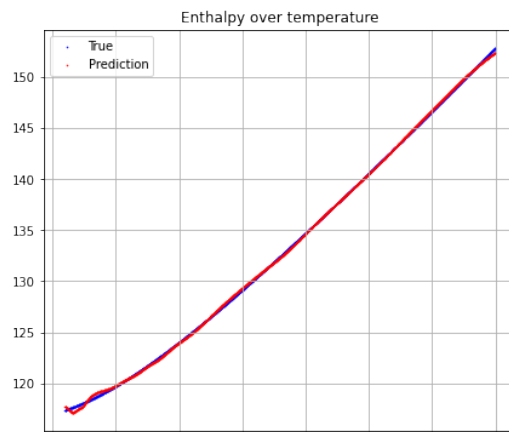
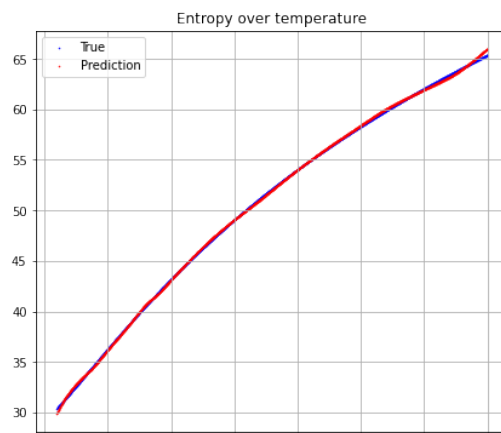
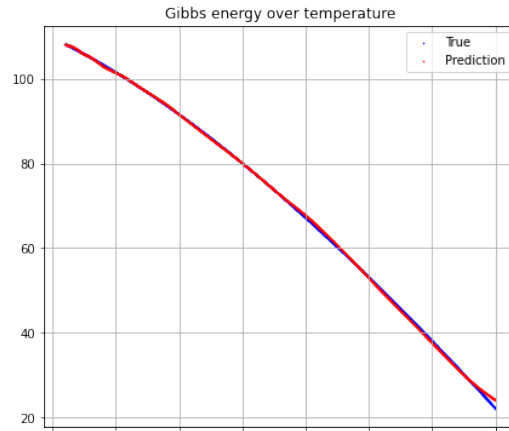
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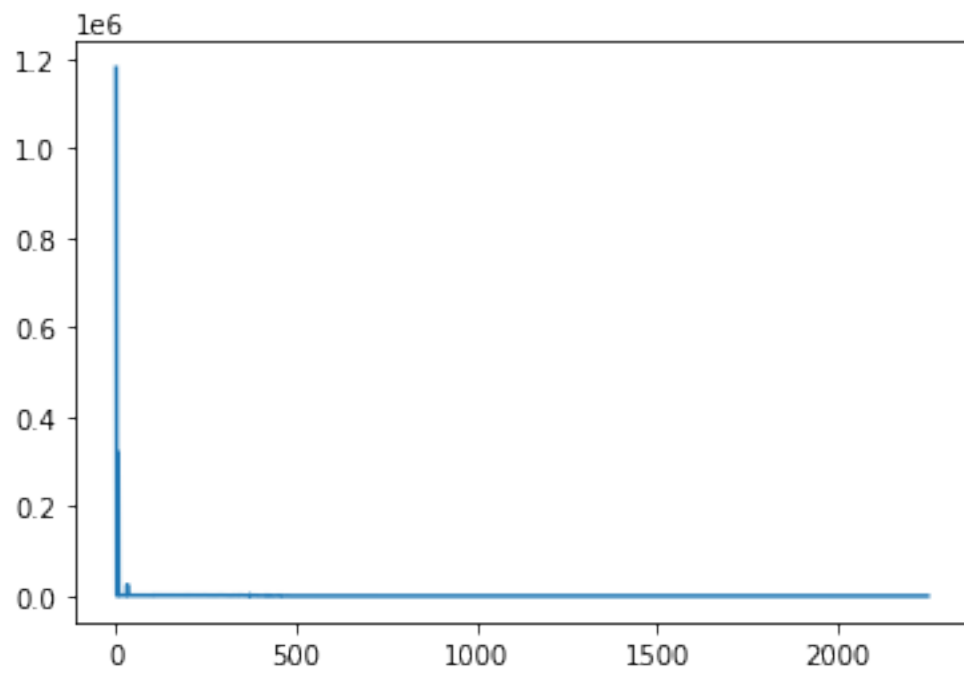
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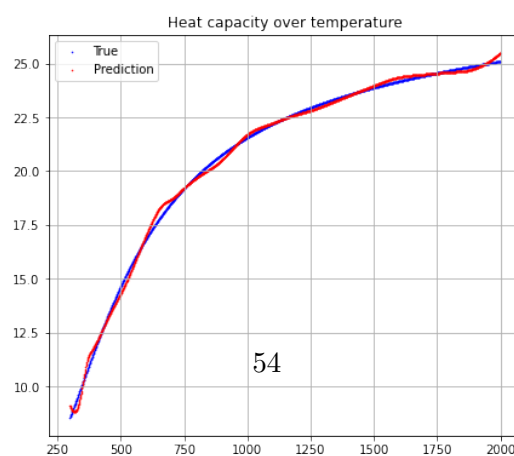
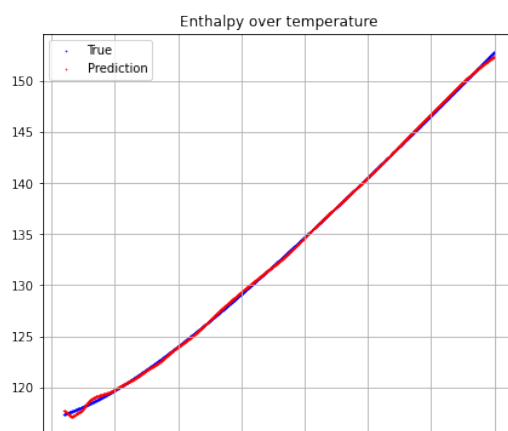
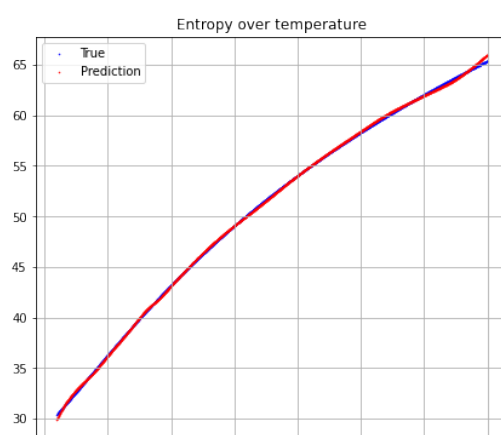
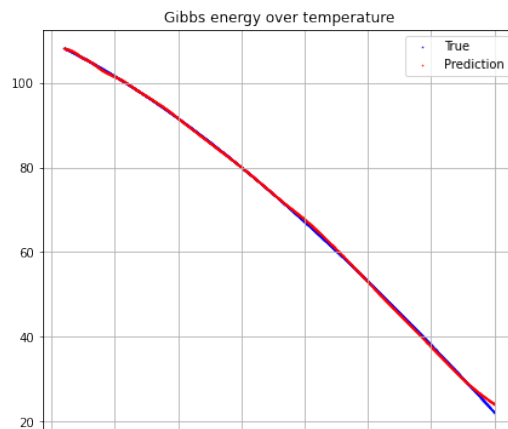
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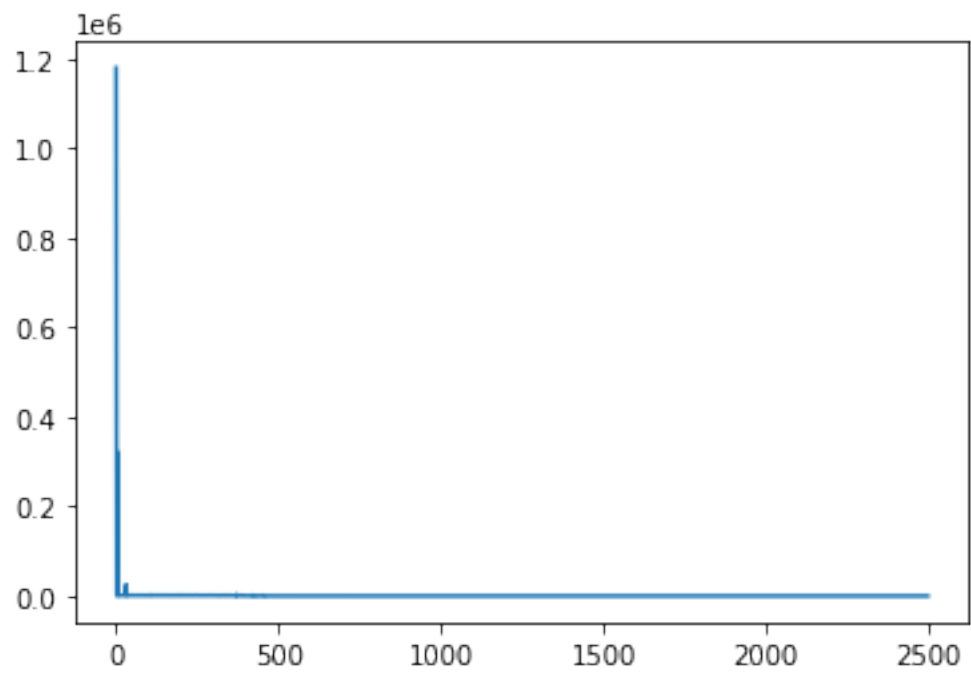
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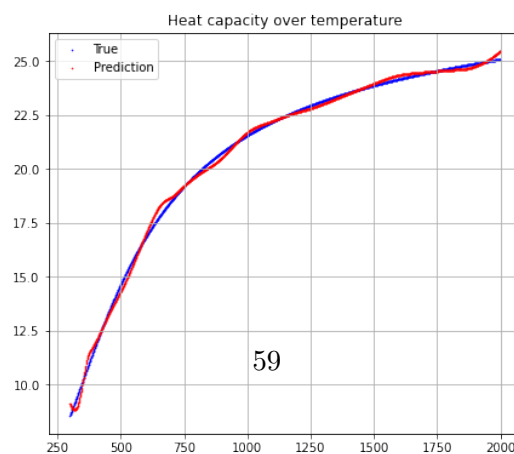
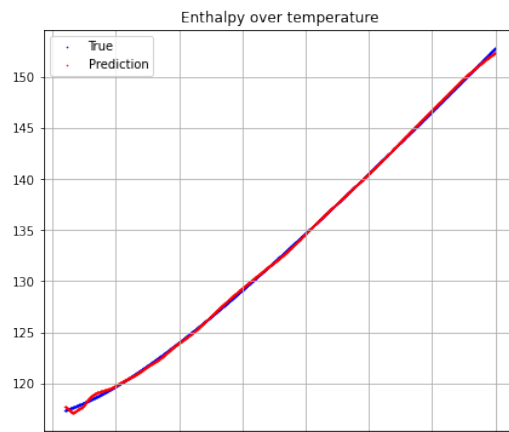
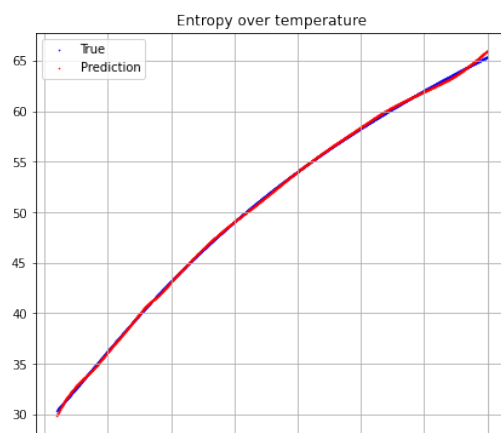
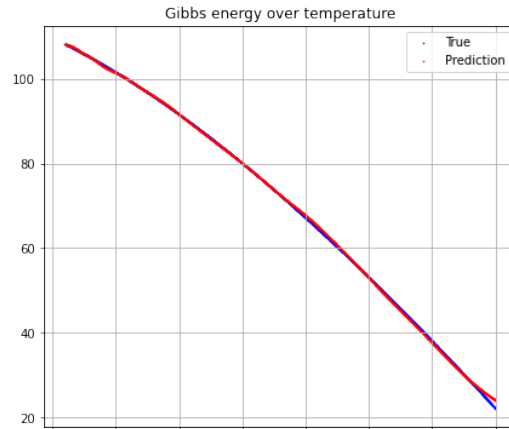
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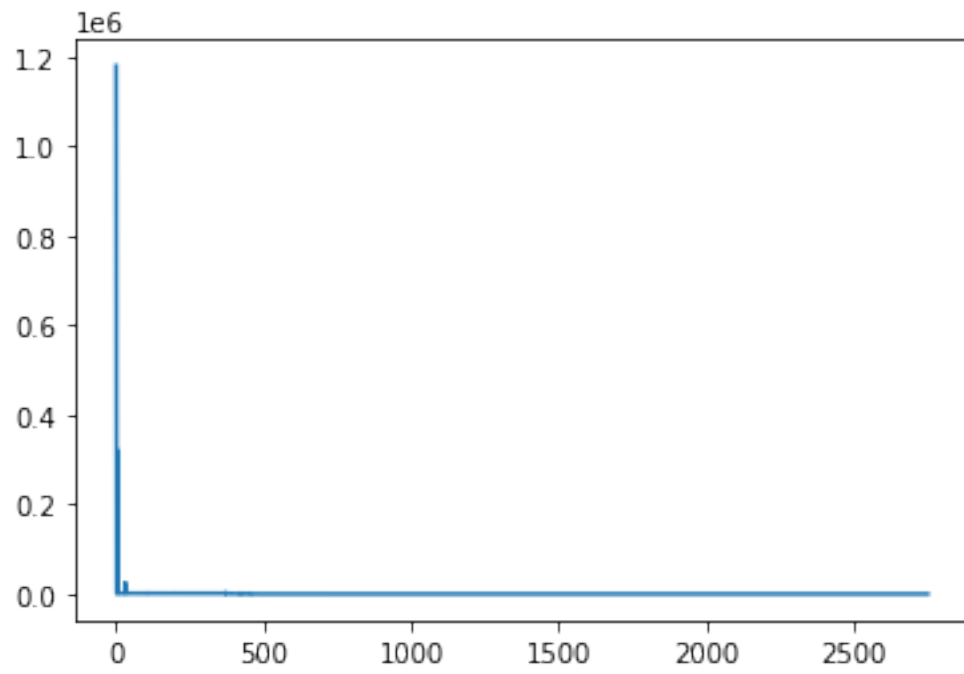
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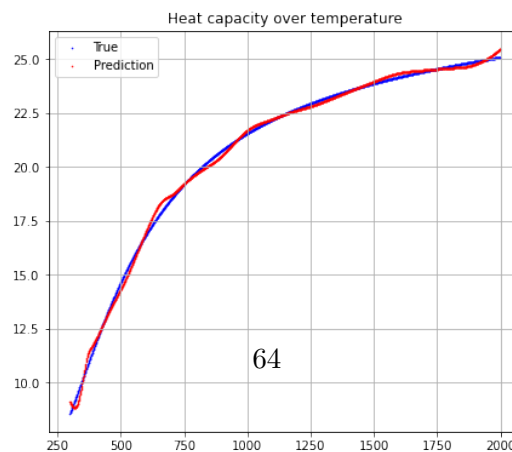
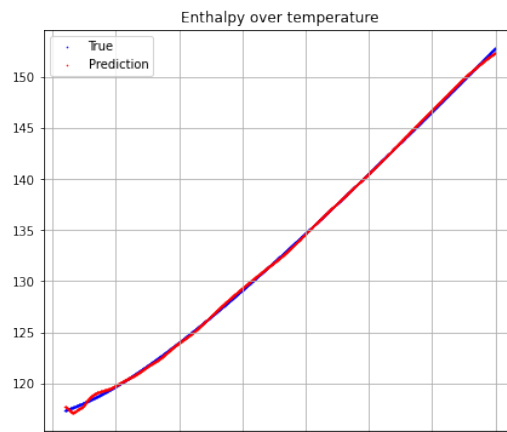
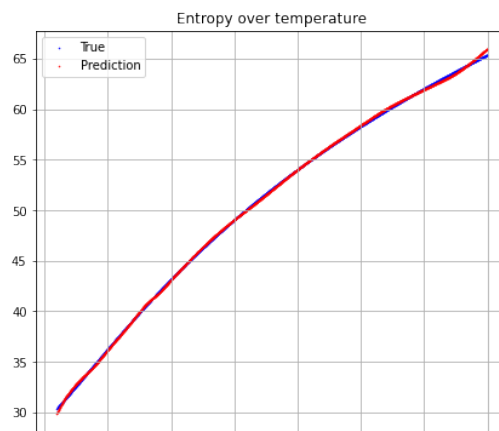
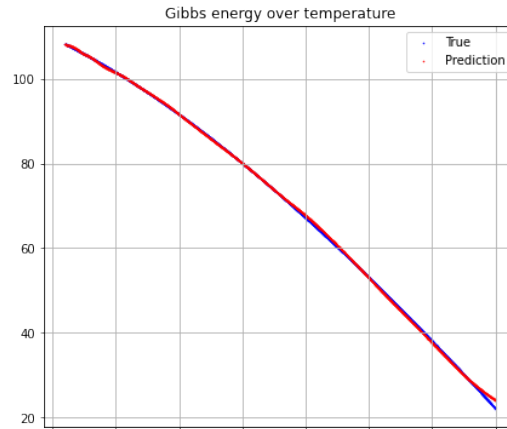
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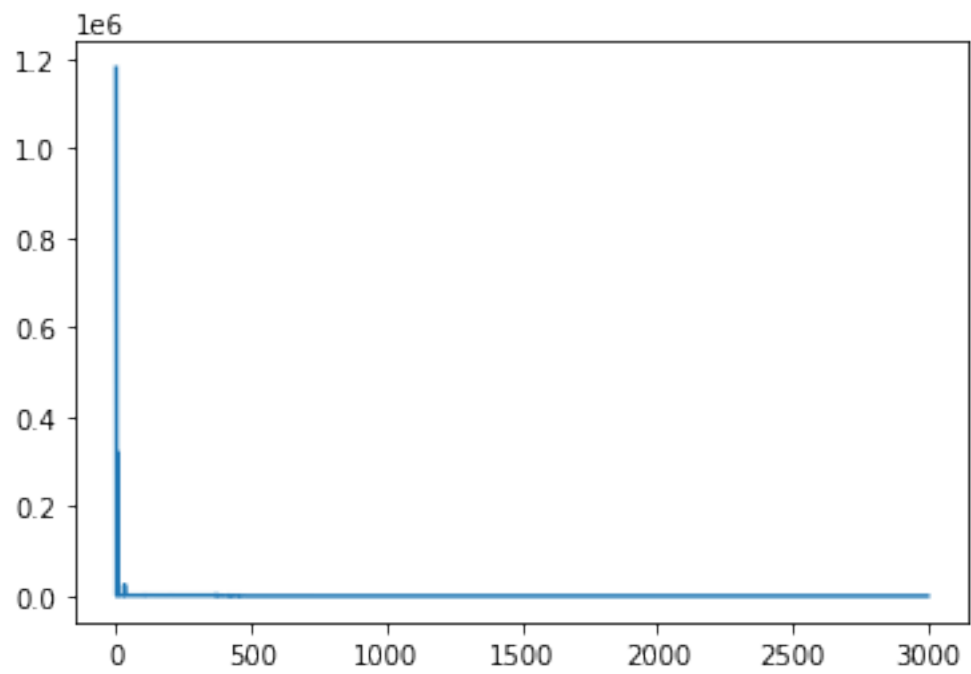
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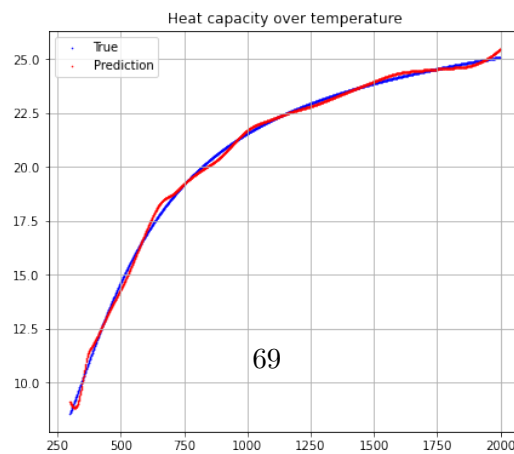
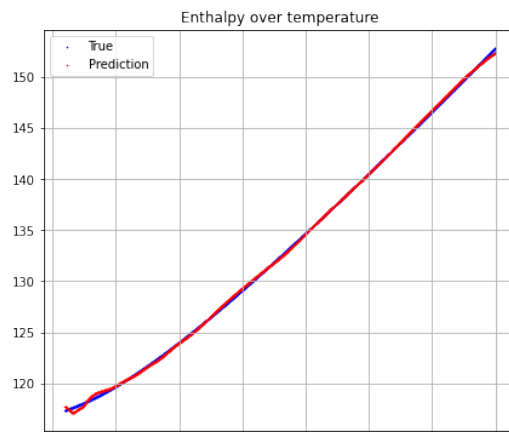
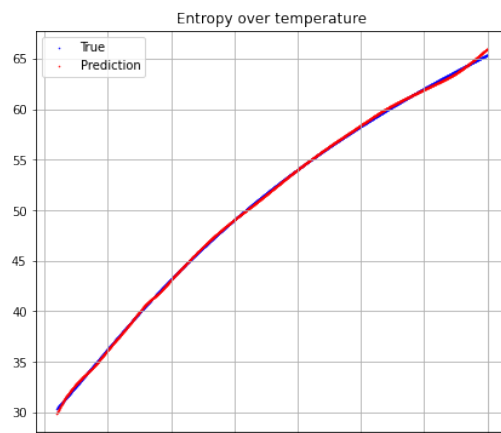
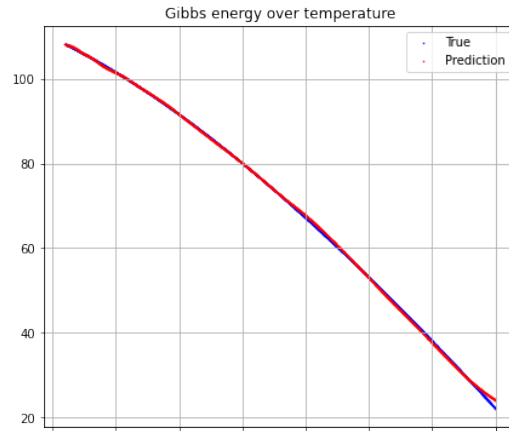
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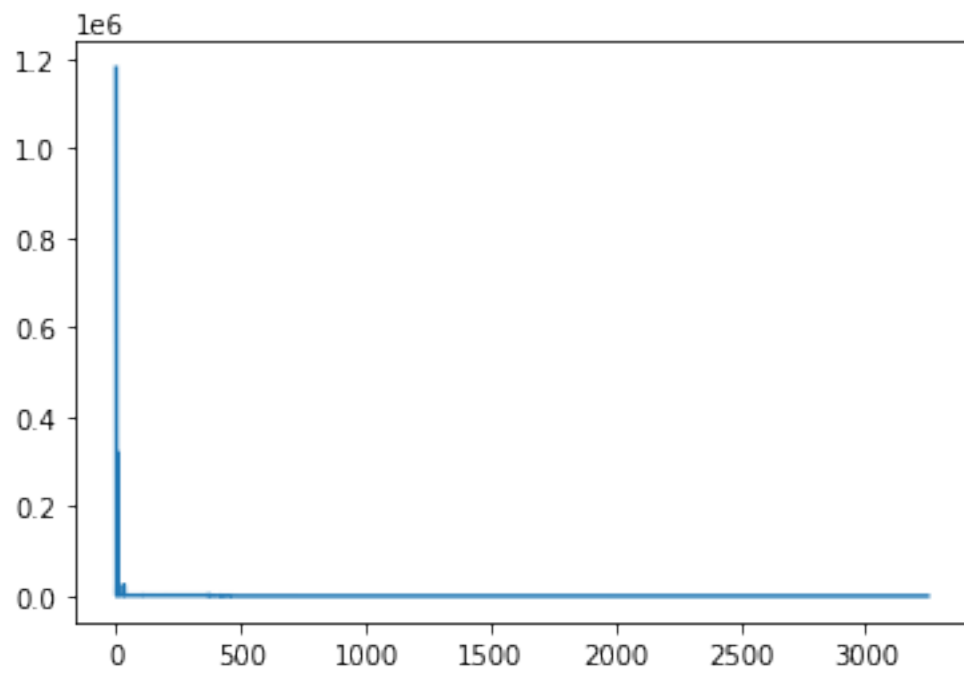
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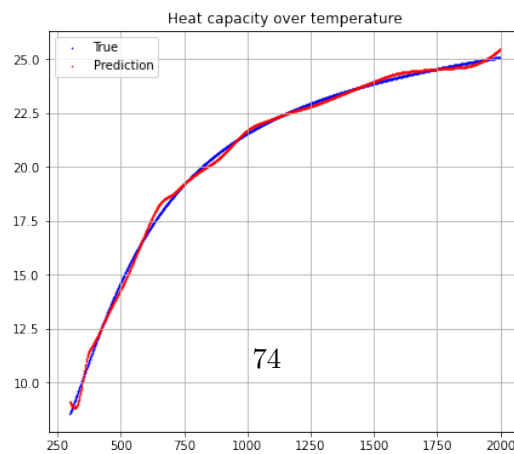
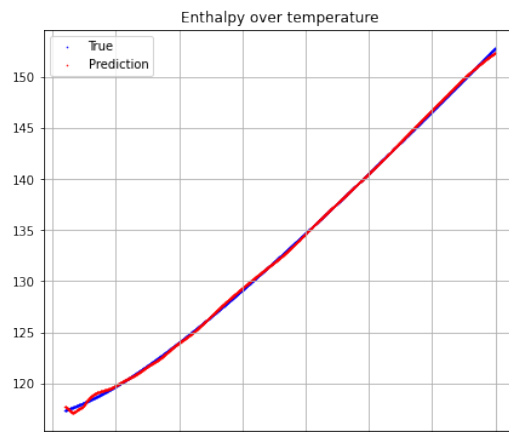
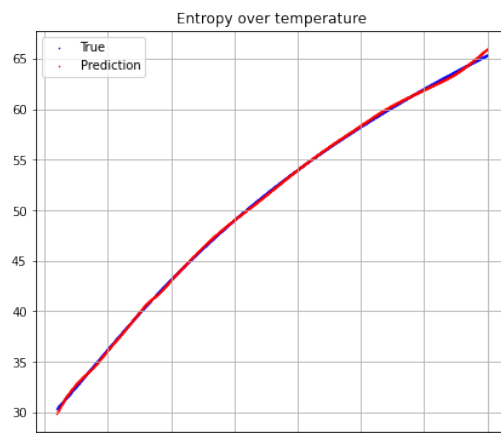
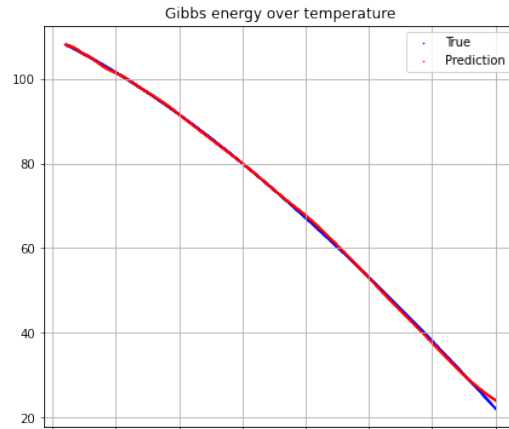
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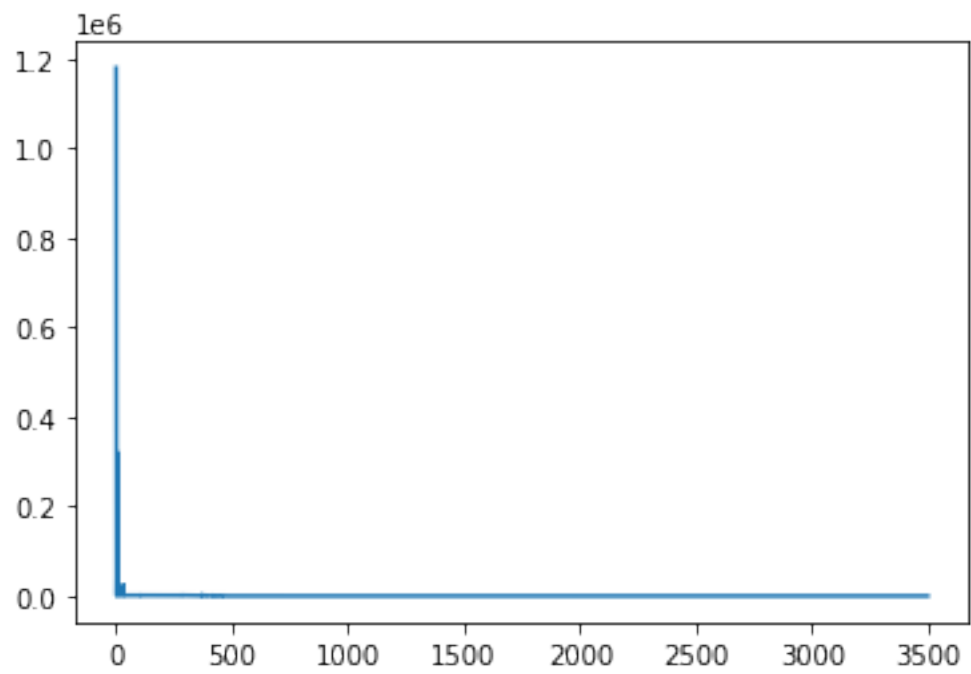
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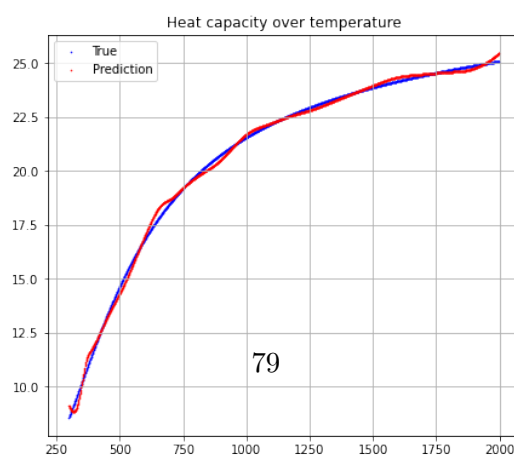
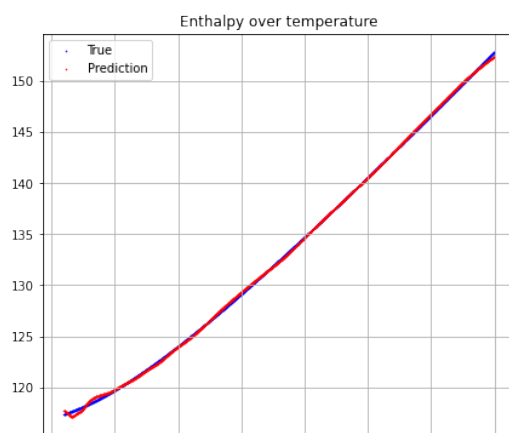
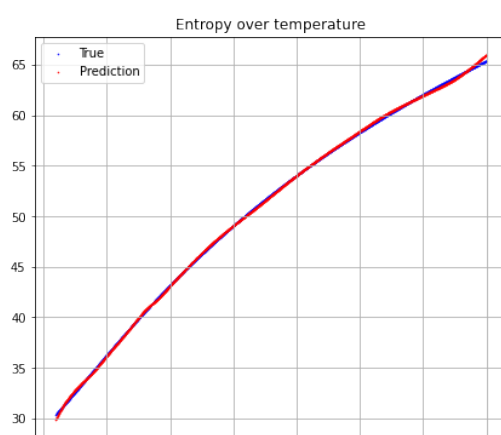
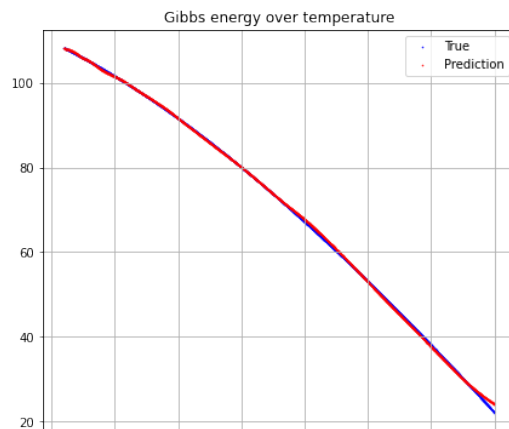
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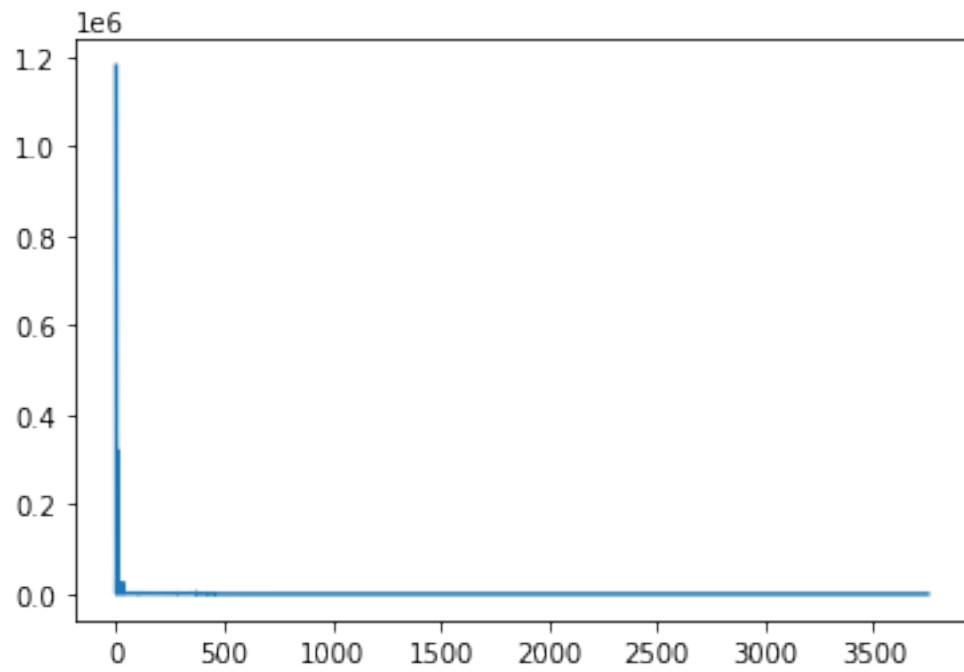
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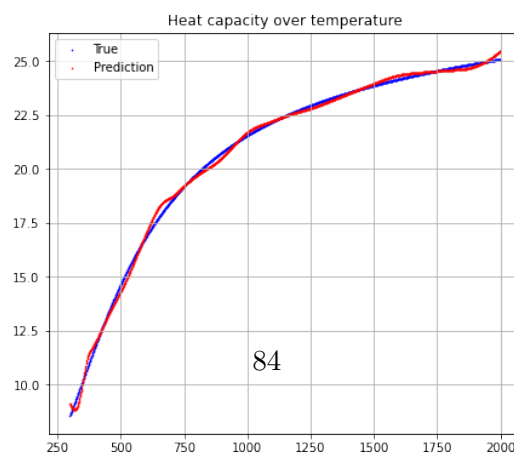
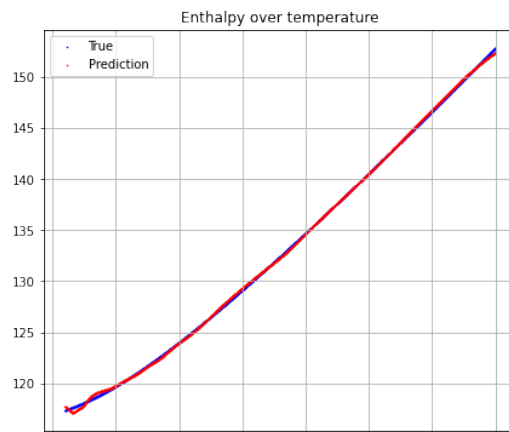
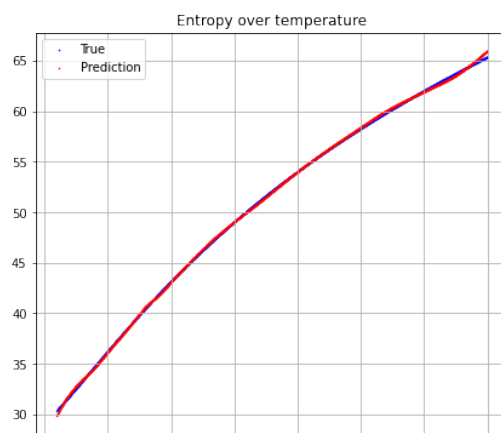
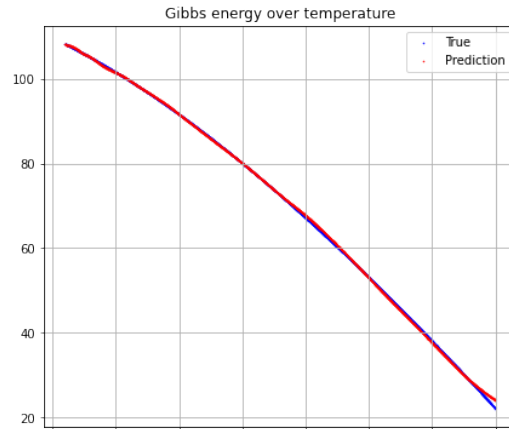
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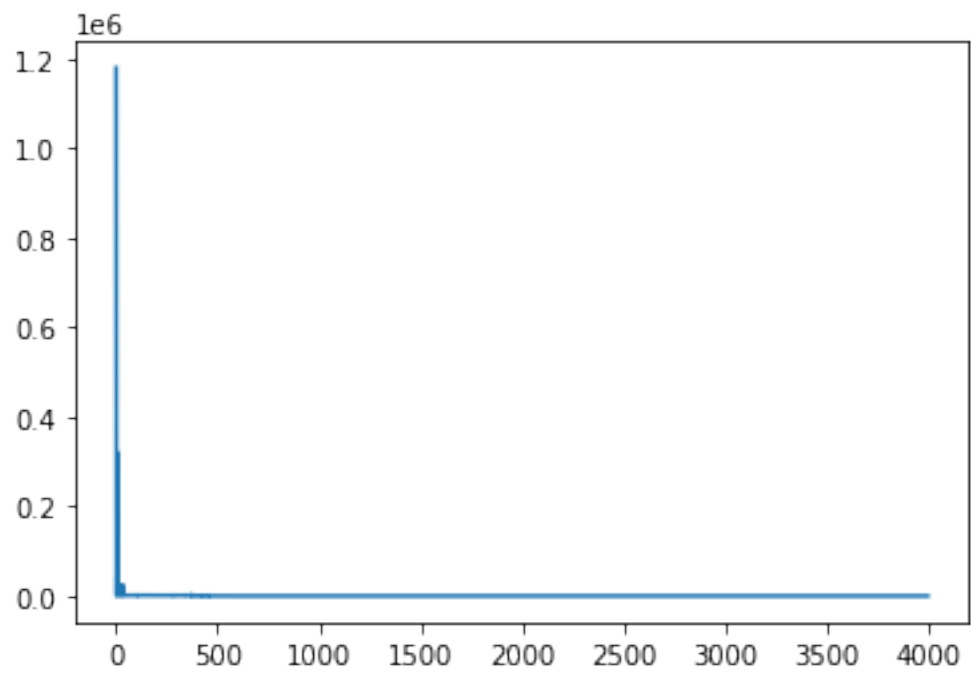
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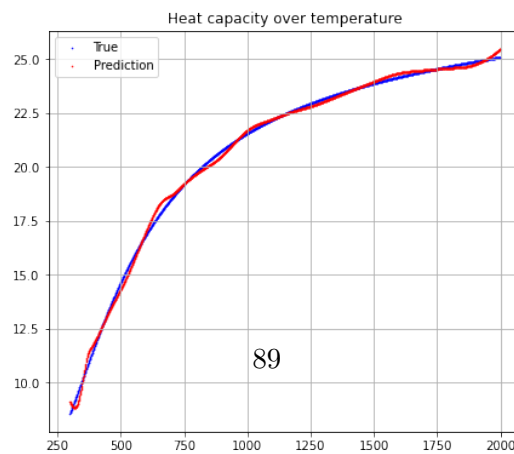
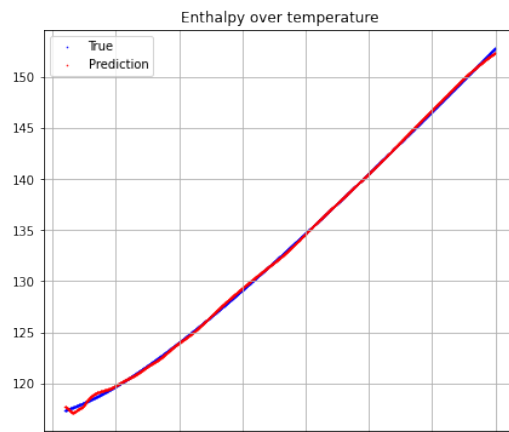
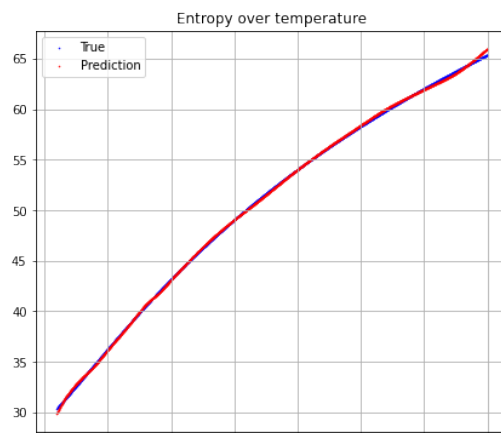
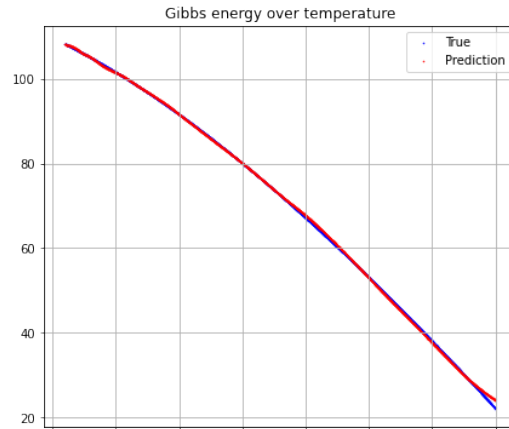
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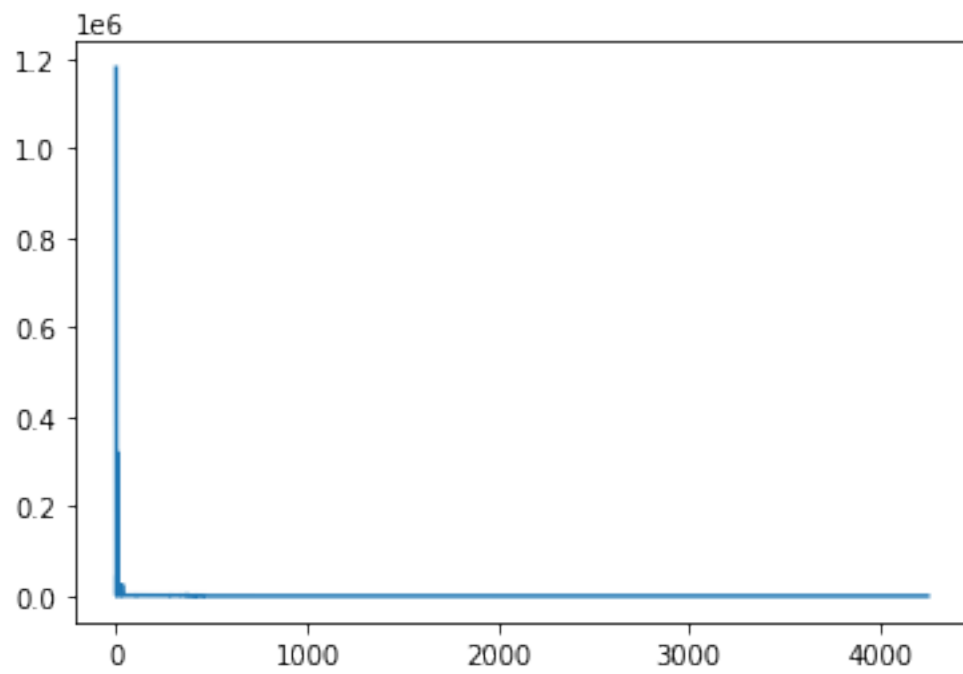
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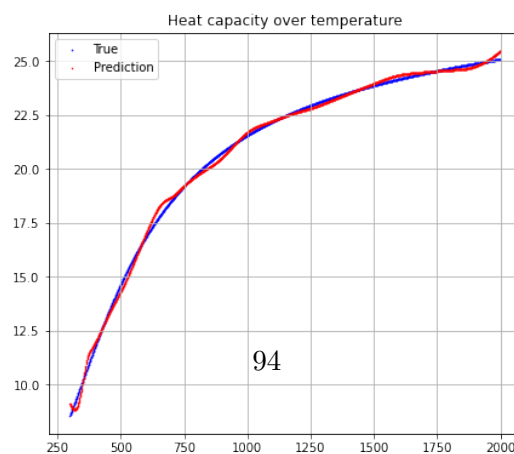
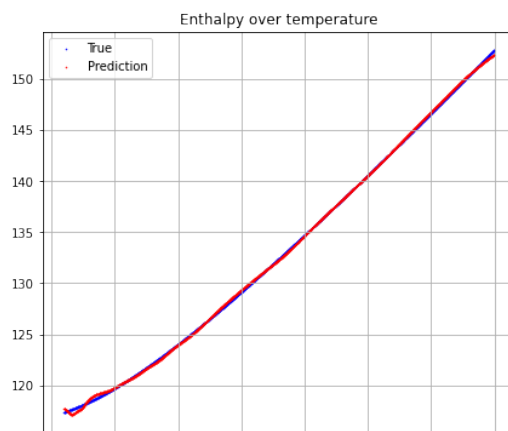
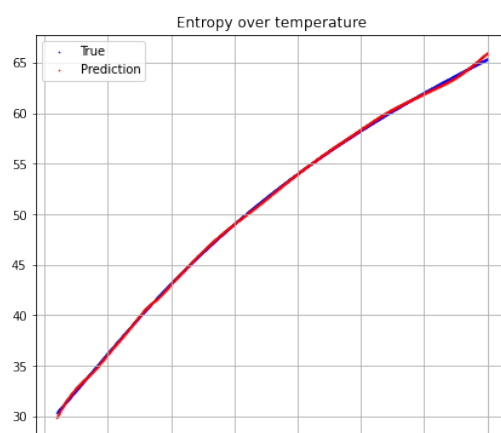
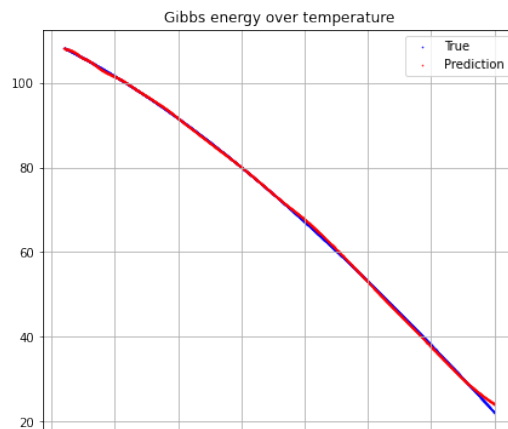
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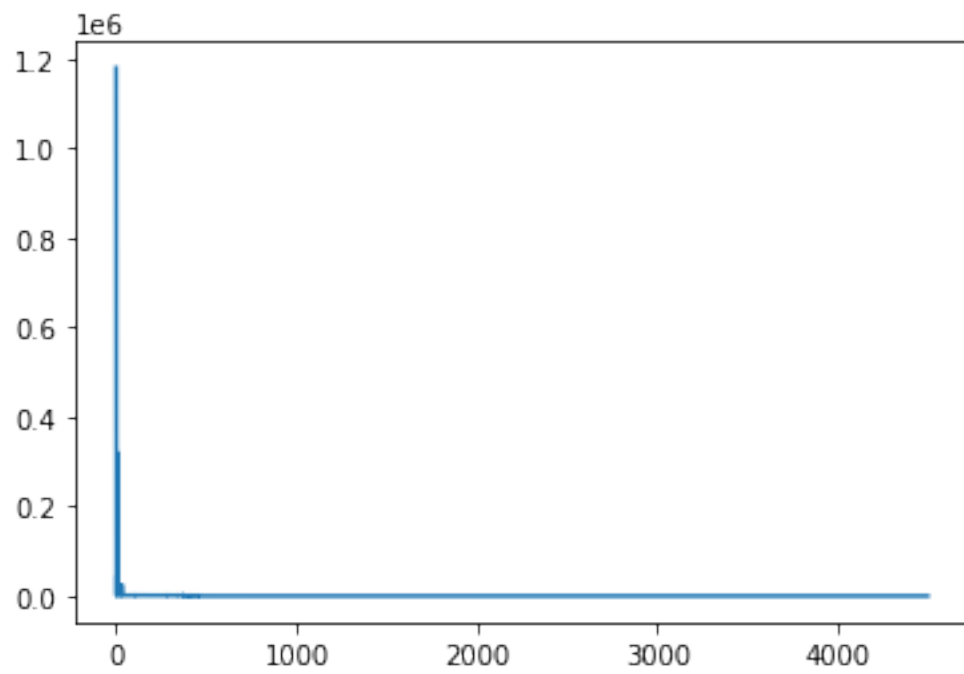
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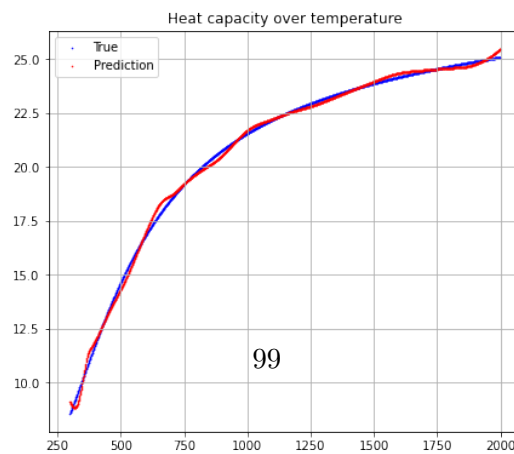
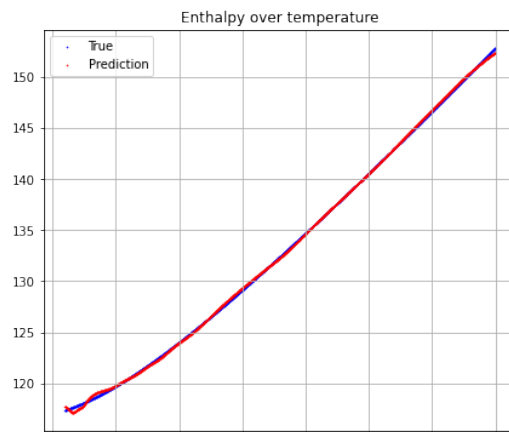
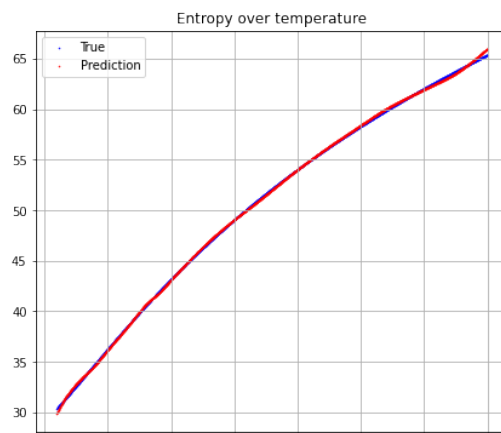
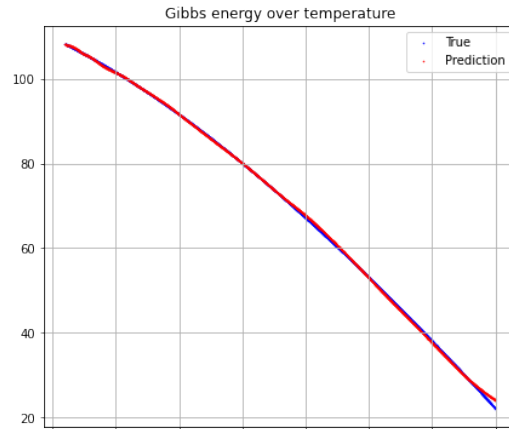
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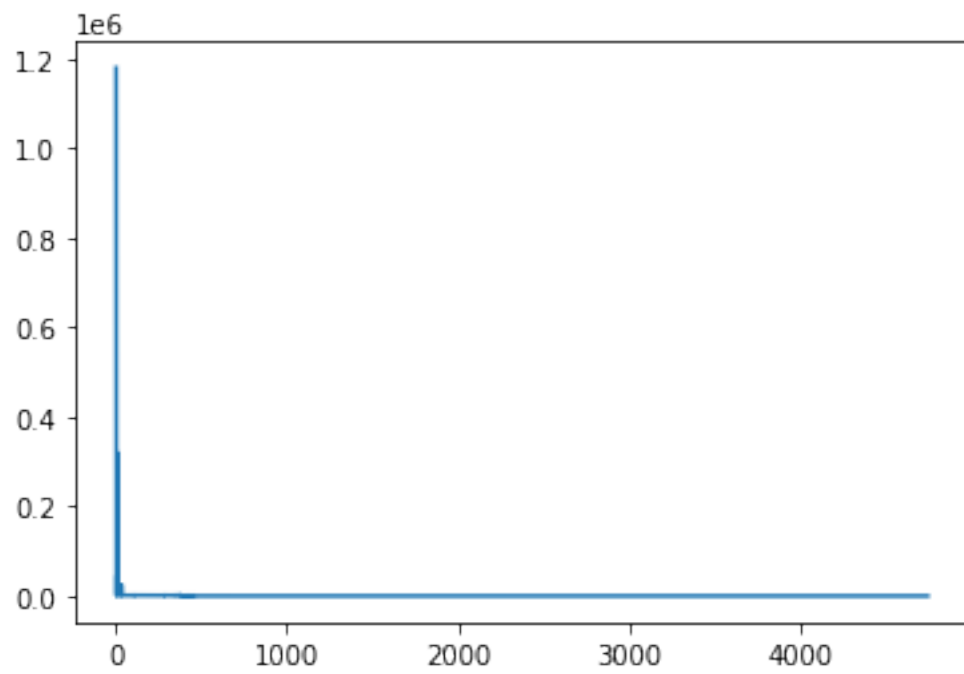
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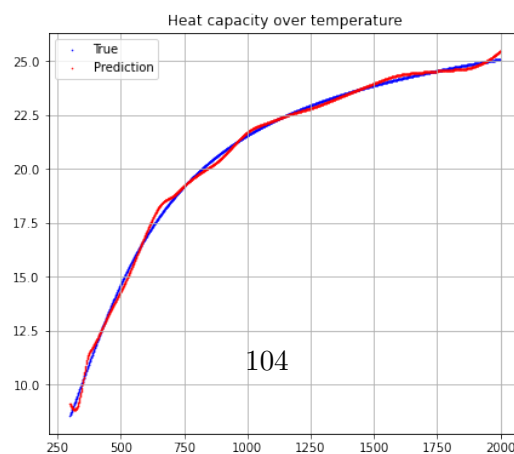
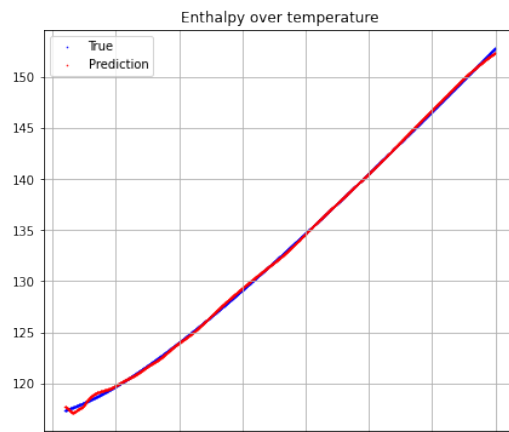
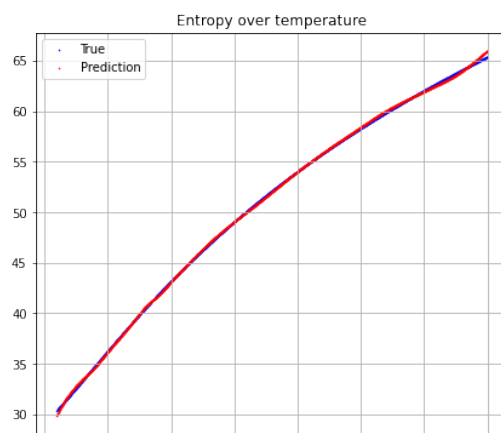
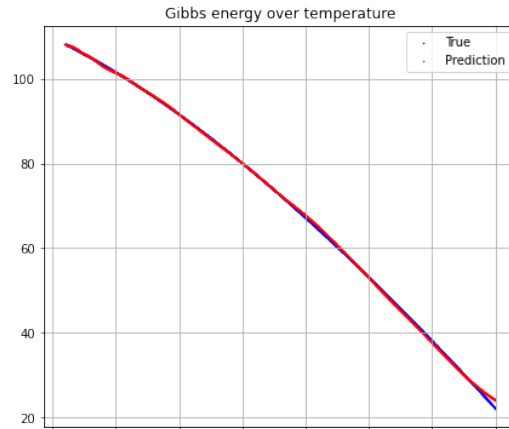
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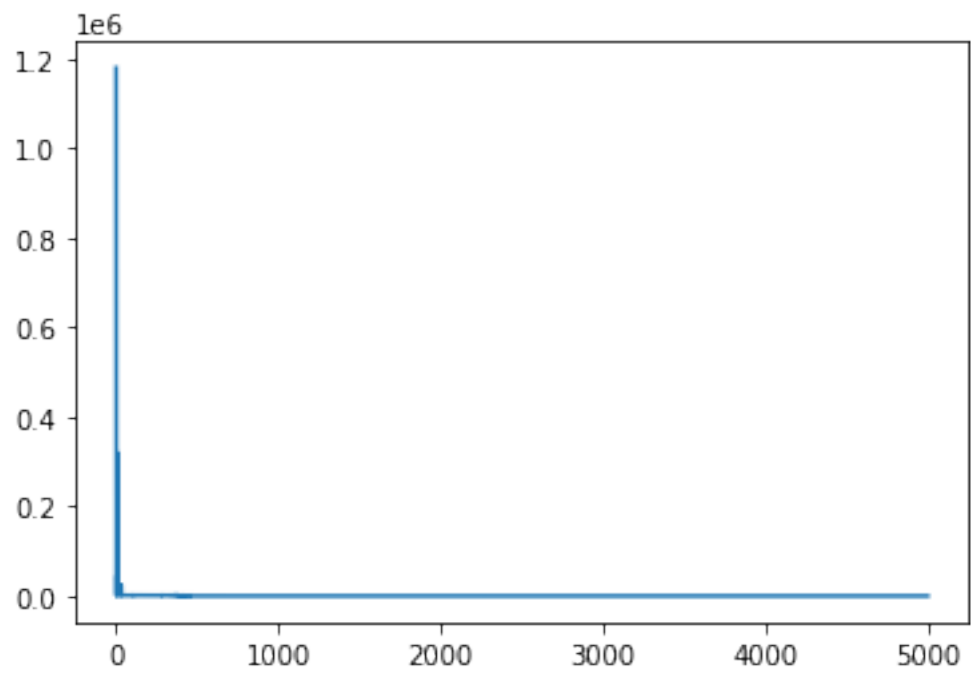
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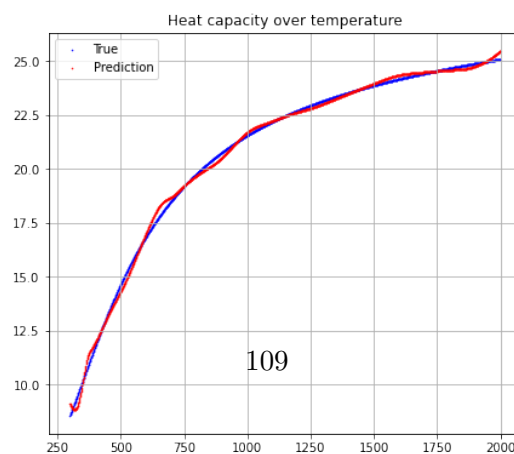
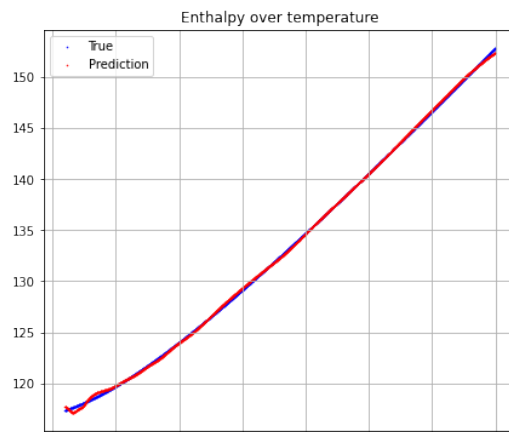
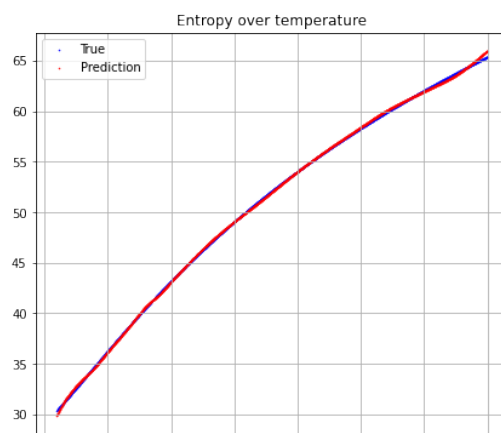
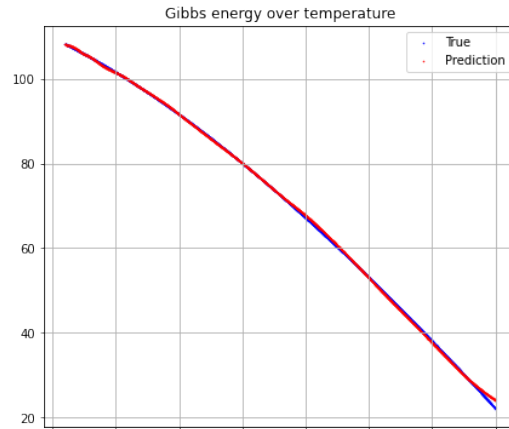
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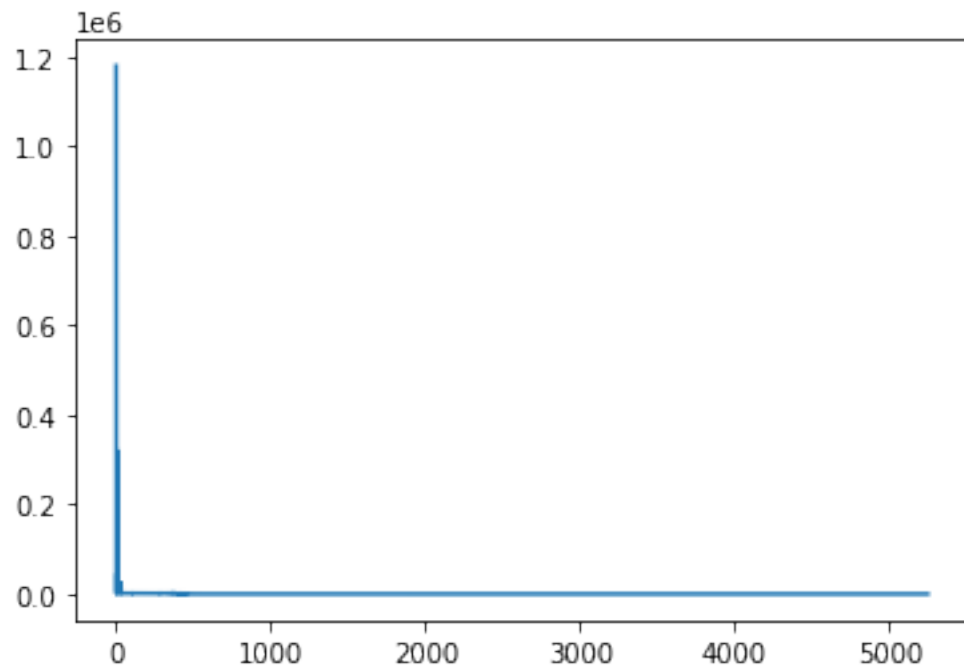
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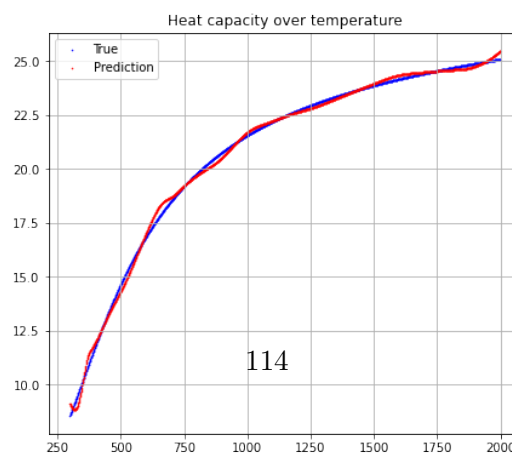
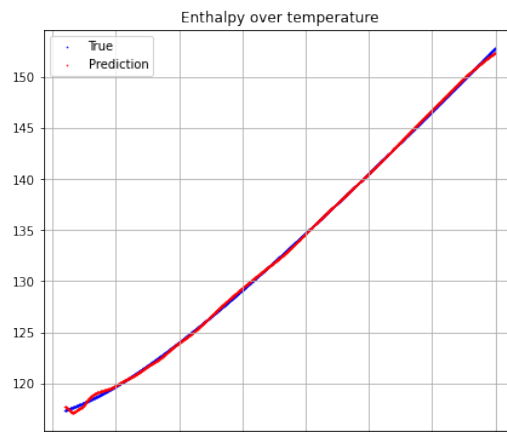
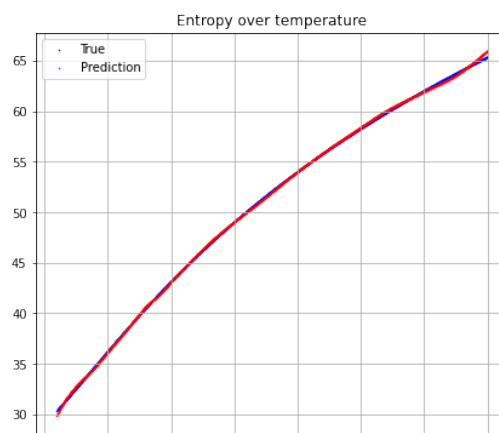
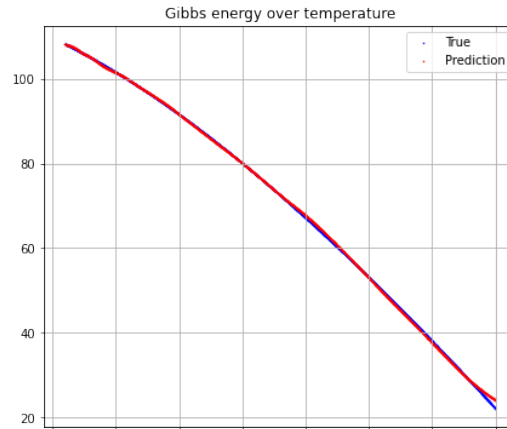
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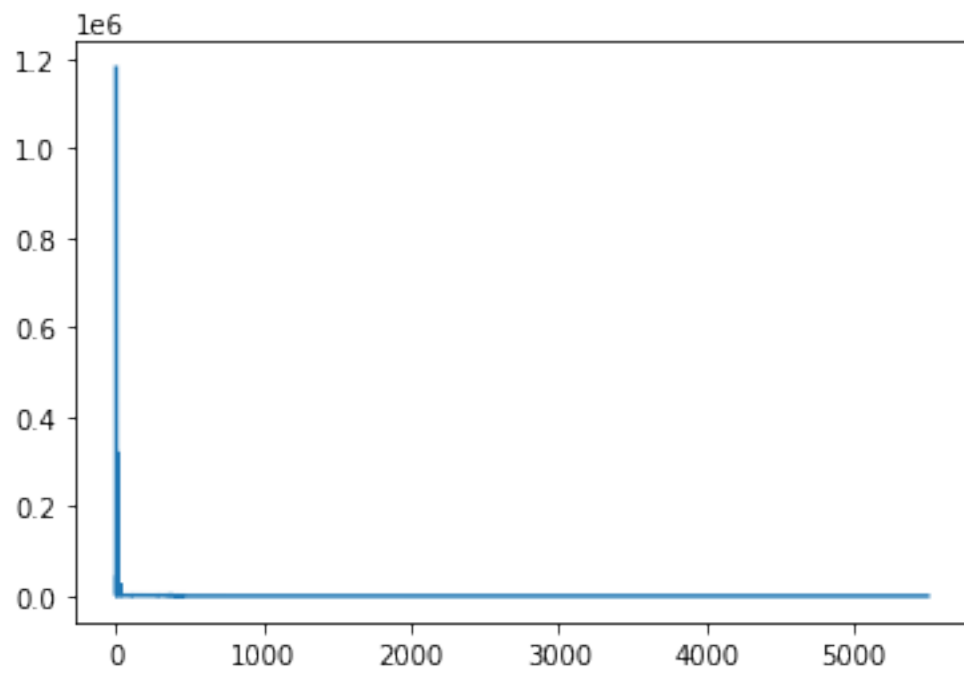
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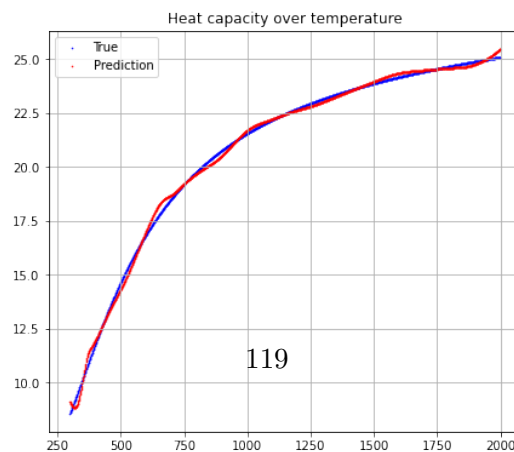
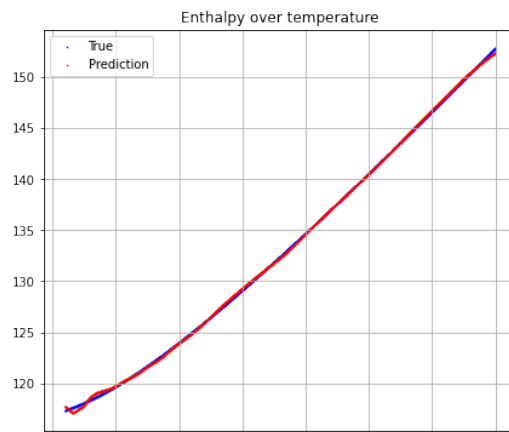
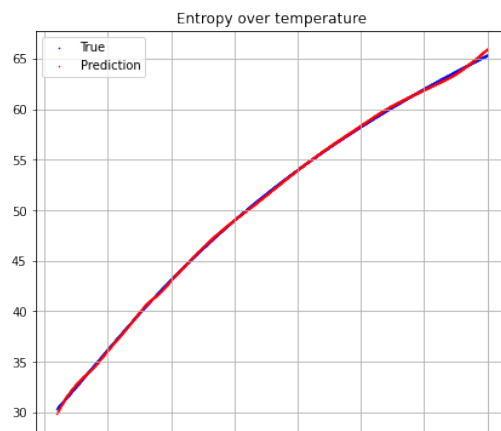
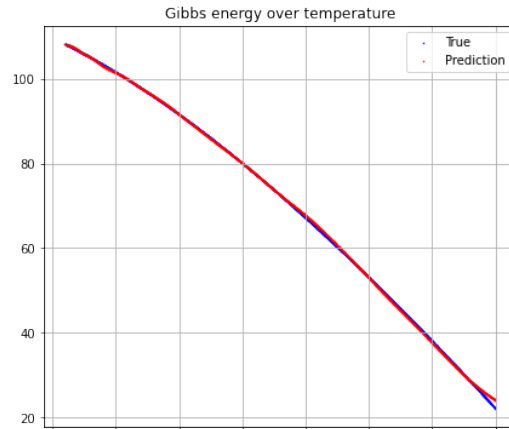
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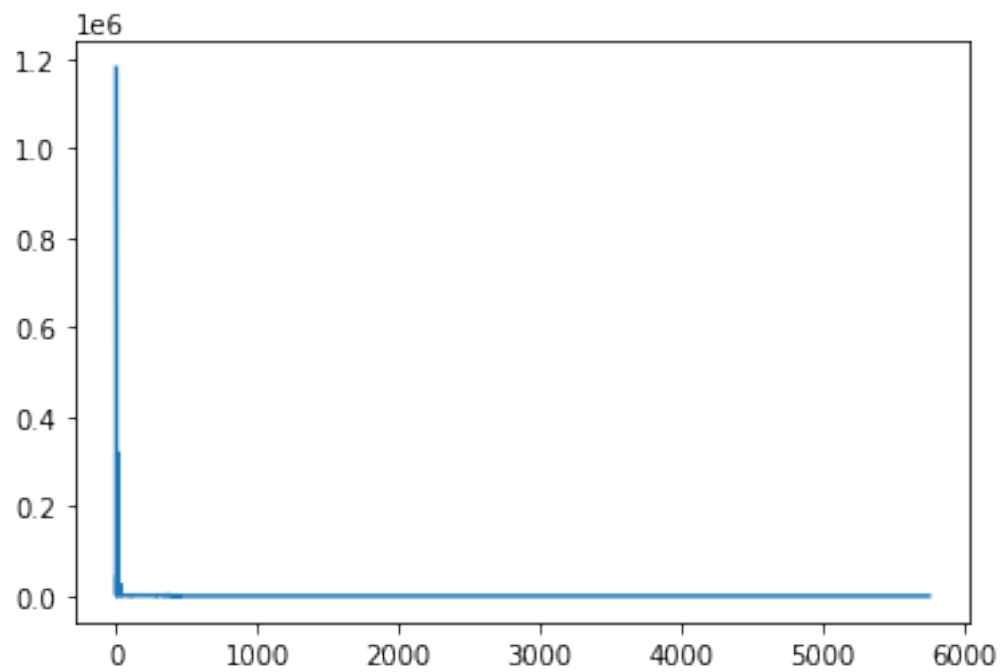
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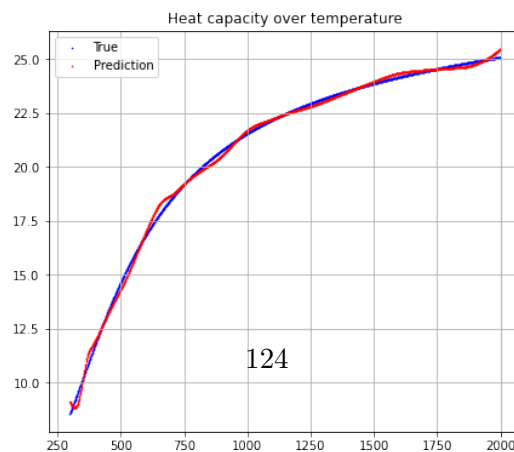
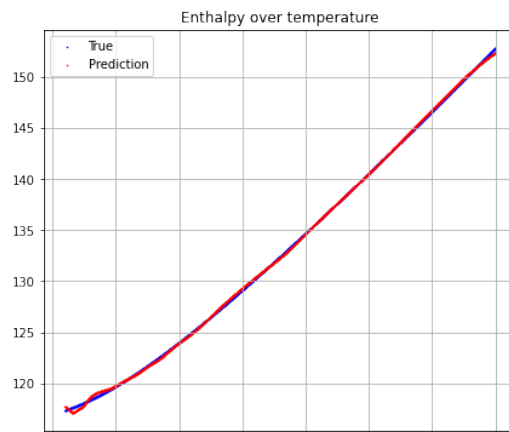
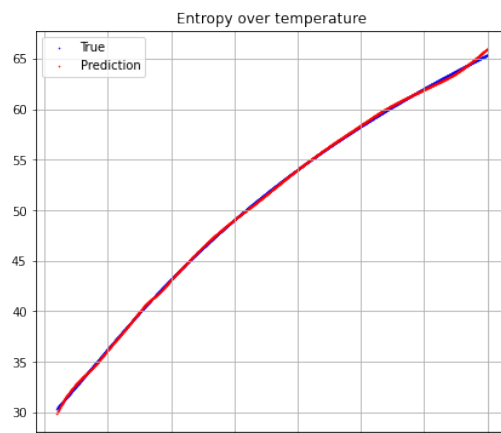
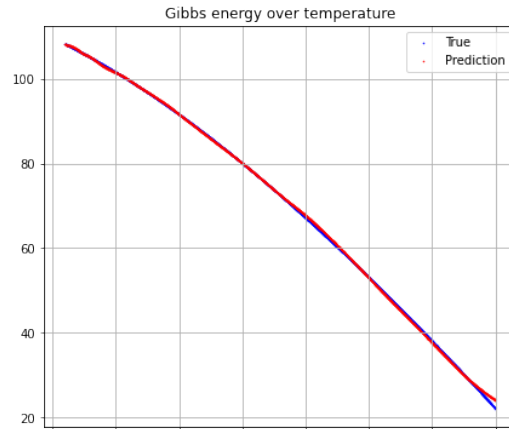
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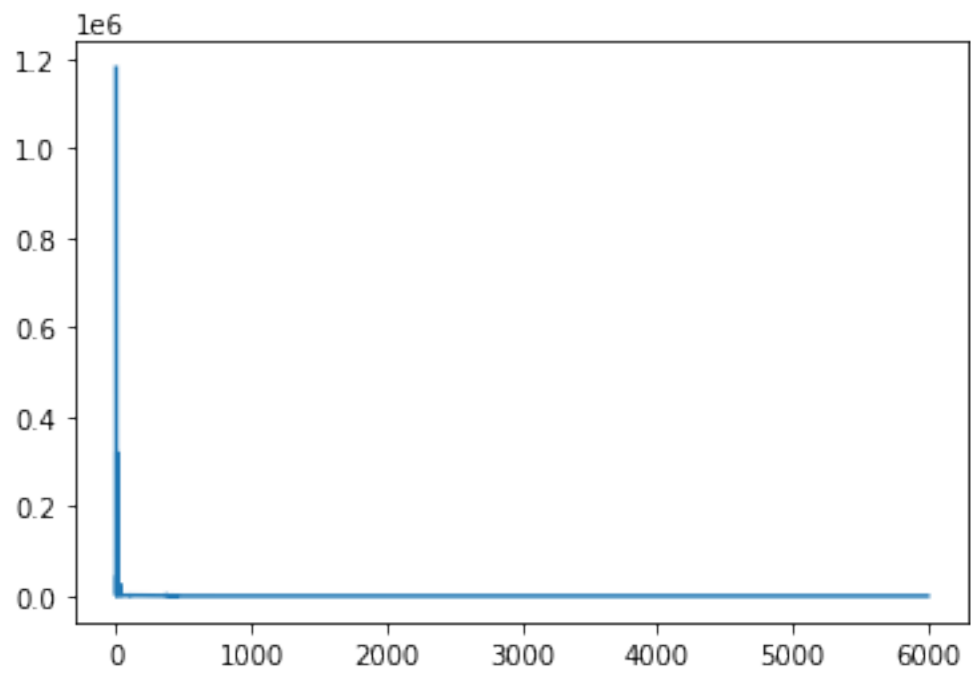
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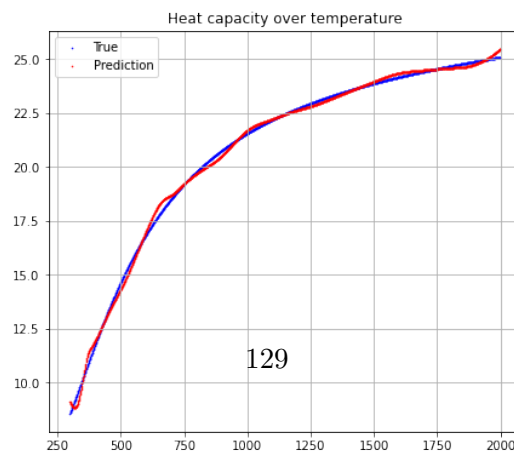
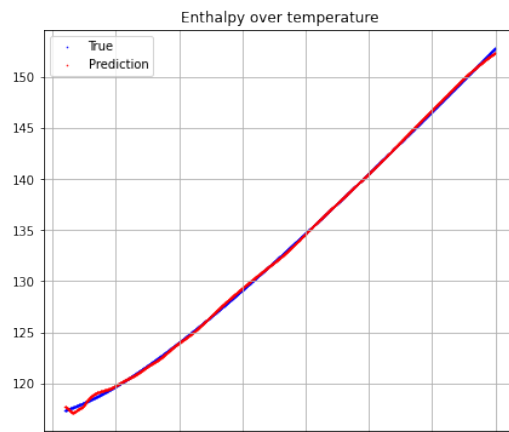
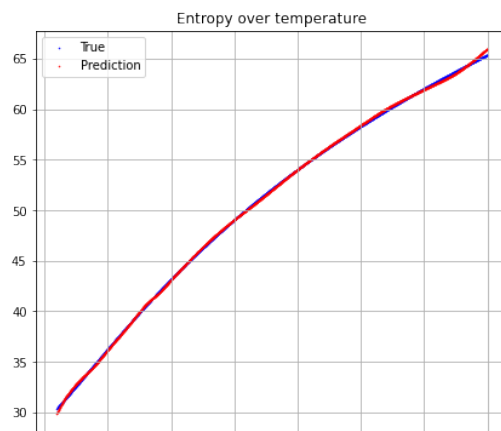
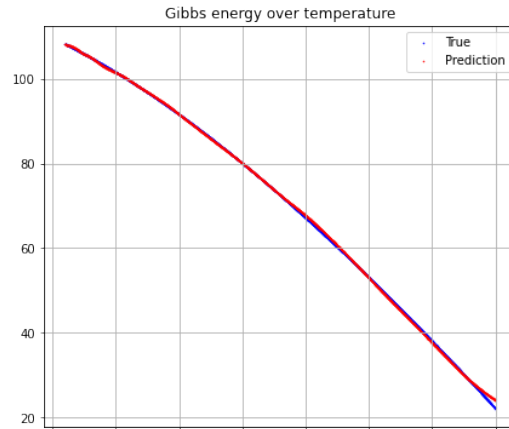
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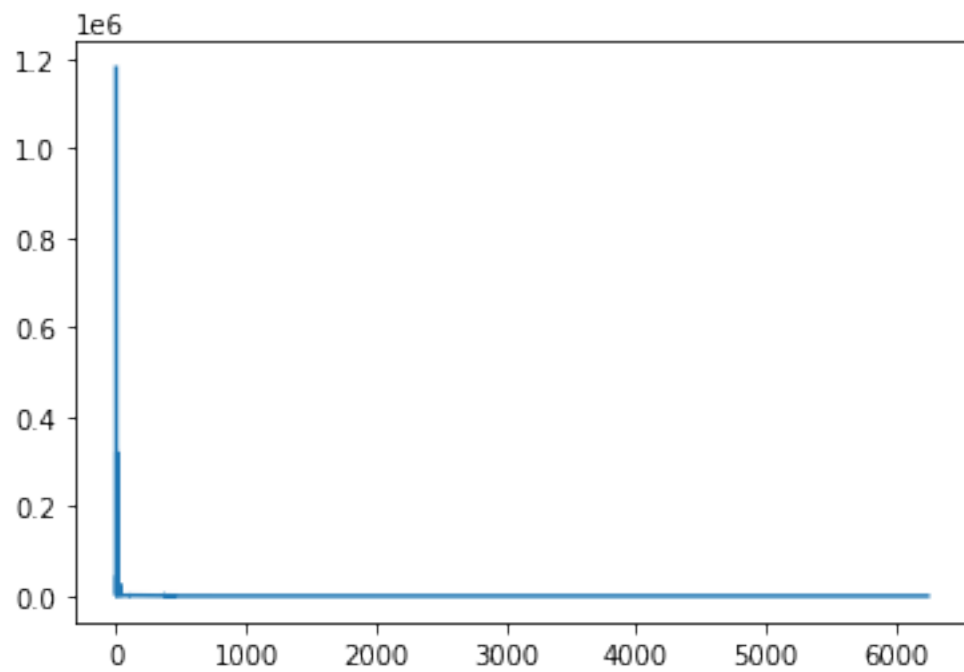
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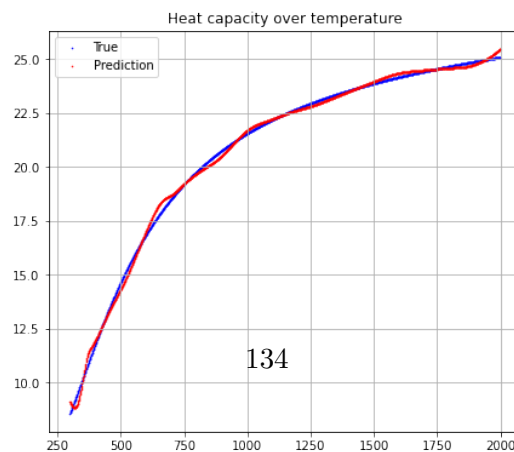
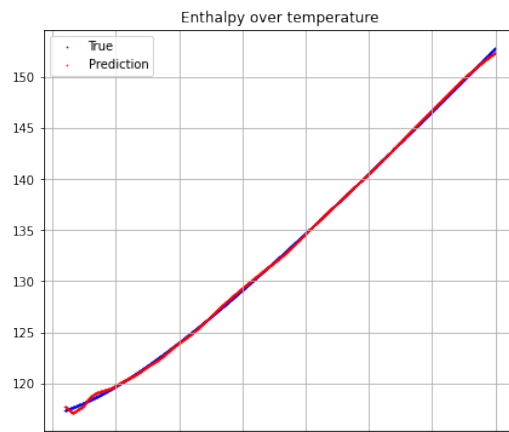
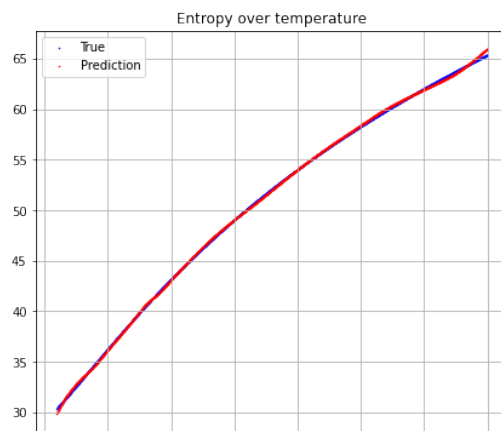
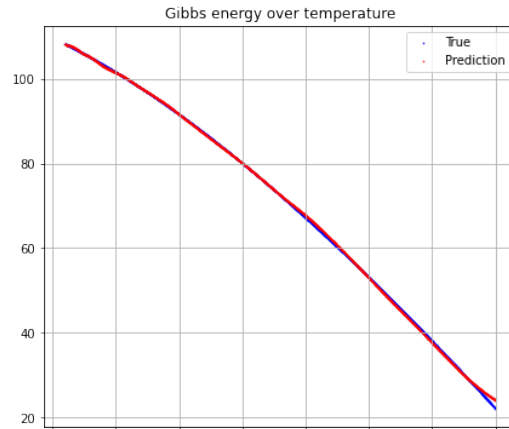
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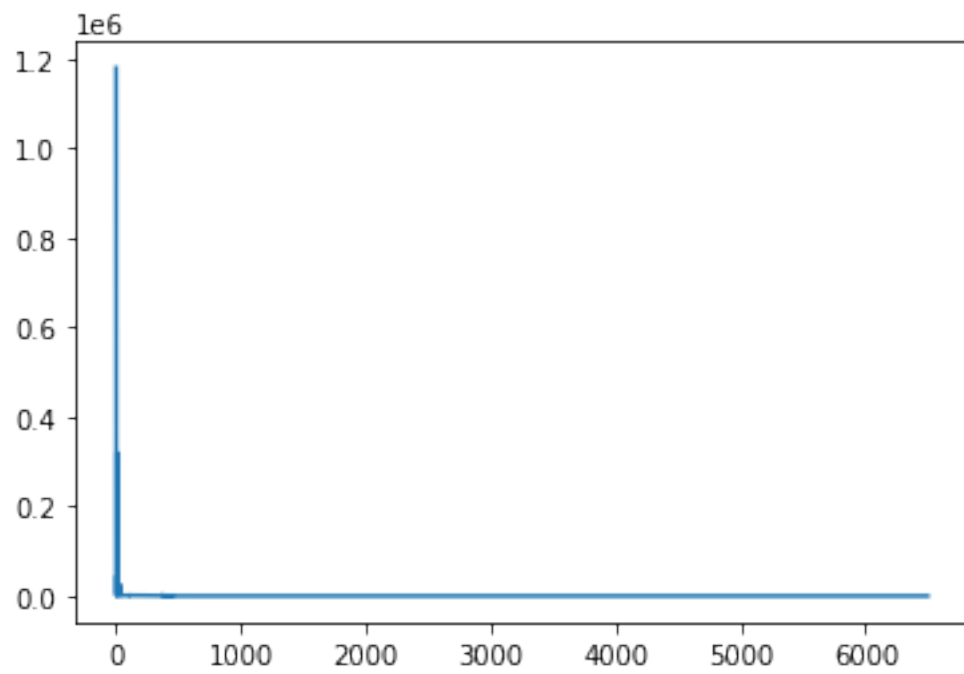
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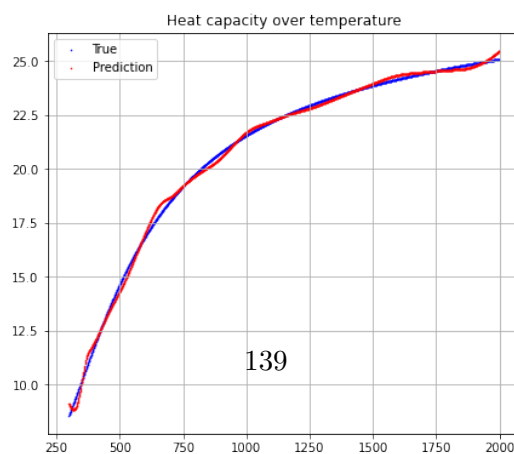
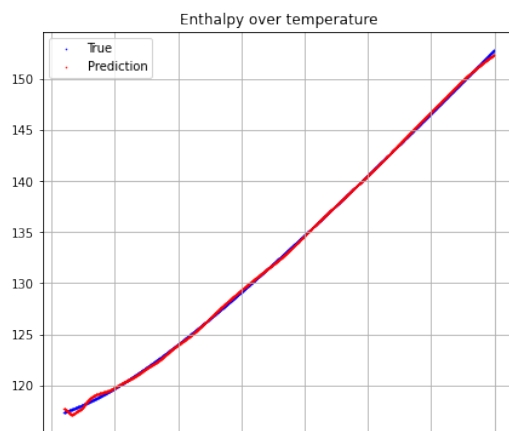
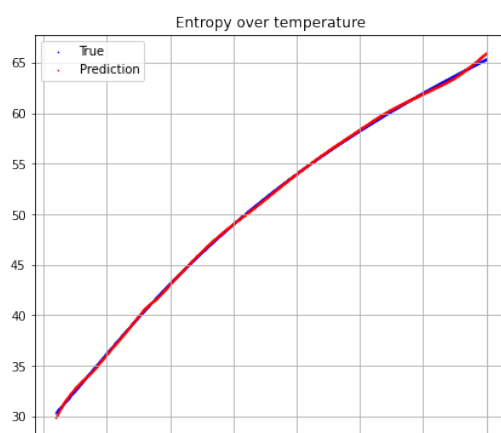
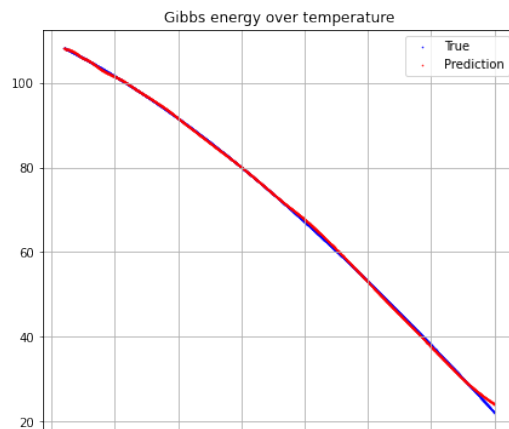
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 -9.159652554259008e-07  
 -124.42752962588987 0.00011397129395579206 0.3218328830599785

6790 : 0.3217364400625229  
 lr: [8.190952912521588e-18]  
 -3.8134808443030533e-07  
 -300.6115788841695 0.00011463764976504767 0.3218314896523953

6800 : 0.3217872828245163  
 lr: [7.790498293267401e-18]  
 -1.6452098379329759e-07  
 -728.1107875893969 0.0001197895030847203 0.321831084638834

6810 : 0.32160715758800507  
 lr: [7.409621848102932e-18]  
 -7.090823990958077e-06  
 -15.6718417334955 0.00011112627134636791 0.32181646808981895

6820 : 0.32179100811481476  
 lr: [7.047366402651213e-18]  
 -1.4539275850568499e-06  
 -68.367199548533 9.940095733669832e-05 0.3218163089454174

6830 : 0.3219541013240814  
 lr: [6.7028215786656915e-18]  
 1.9055240008295799e-06  
 55.957128698954534 0.00010662765175336755 0.32181060999631883

6840 : 0.3218682259321213  
 lr: [6.375121506173517e-18]  
 1.5223512844163545e-06  
 65.92184158791719 0.00010035620021245718 0.32180784806609153

6850 : 0.32188697159290314  
 lr: [6.063442647471843e-18]  
 4.257474626813616e-08  
 2191.824887421951 9.331638844617568e-05 0.3218193228542805

6860 : 0.3218664228916168  
 lr: [5.767001727508669e-18]  
 3.5236684643492408e-06  
 28.214372106990055 9.94180932348157e-05 0.32182673320174215

6870 : 0.3218238949775696  
 lr: [5.4850537654471014e-18]  
 -2.56360793600277e-07  
 -384.7098450099654 9.862452117259431e-05 0.3218261797726154

6880 : 0.32182830572128296  
 lr: [5.2168902024661655e-18]  
 1.5326908656529018e-06  
 57.79777953999494 8.858612875597043e-05 0.3218202295899391

6890 : 0.32173265516757965  
 lr: [4.961837121093202e-18]  
 -1.121844564165388e-06  
 -73.81744267045131 8.281169680043596e-05 0.3218142527341843

6900 : 0.32179637253284454  
 lr: [4.719253551592864e-18]  
 3.3336026327950615e-06  
 23.850691269003505 7.950872720833227e-05 0.32180570274591447

6910 : 0.3220278471708298  
 lr: [4.488529861156546e-18]  
 4.892142451539331e-06  
 16.815890319772134 8.226573089378656e-05 0.3218034255504608

6920 : 0.3218989819288254  
 lr: [4.2690862218441145e-18]  
 4.270247050694057e-06  
 20.101733601172835 8.583936862424592e-05 0.3217983043193817

6930 : 0.32190951704978943  
 lr: [4.0603711534277845e-18]  
 4.680181036190111e-07  
 204.0431762344516 9.549590039764771e-05 0.321803023815155

6940 : 0.3217446058988571  
 lr: [3.861860137476157e-18]  
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-124.14863430029602 0.0001048813383452206 0.32180222511291506

6950 : 0.3218635022640228

lr: [3.673054299195511e-18]

6.157220626363949e-06

17.872849973679468 0.00011004708050984758 0.3218011969327927

6960 : 0.3217877894639969

lr: [3.493479153715707e-18]

3.860921275858976e-06

26.61442259115579 0.00010275619042689518 0.3218046501278877

6970 : 0.3218614310026169

lr: [3.32268341367e-18]

6.386211940220424e-08

1655.5009586165888 0.00010572379988963618 0.3217979174852371

6980 : 0.32191120088100433

lr: [3.16023785507213e-18]

4.875720763693051e-06

20.704485965895984 0.00010094929212551041 0.32178809493780136

6990 : 0.32177312672138214

lr: [3.0057342386405243e-18]

3.3664460084876236e-07

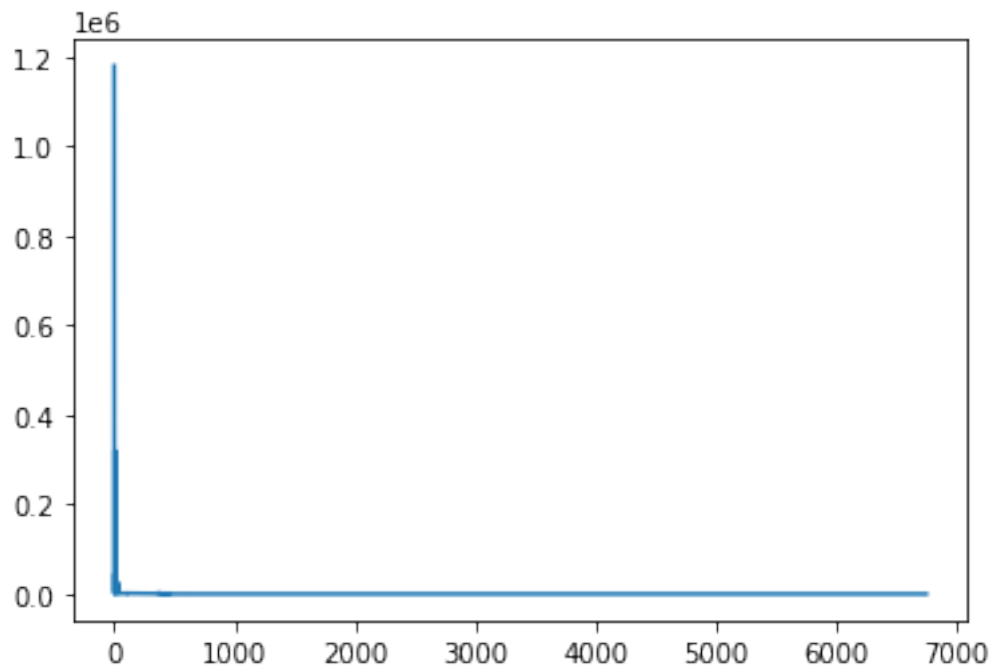
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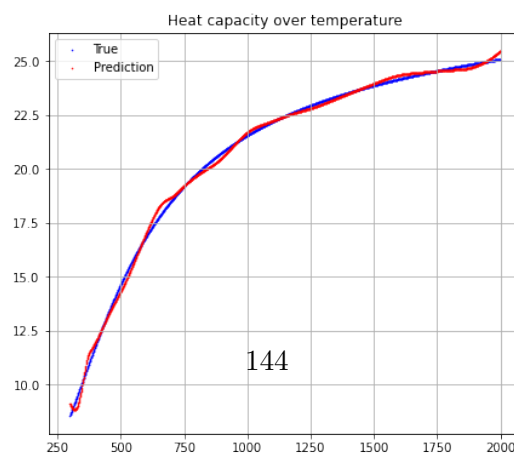
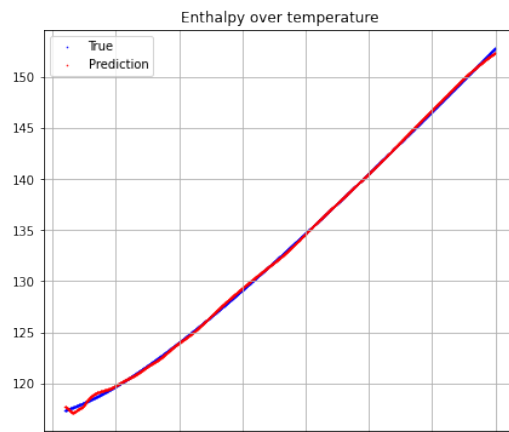
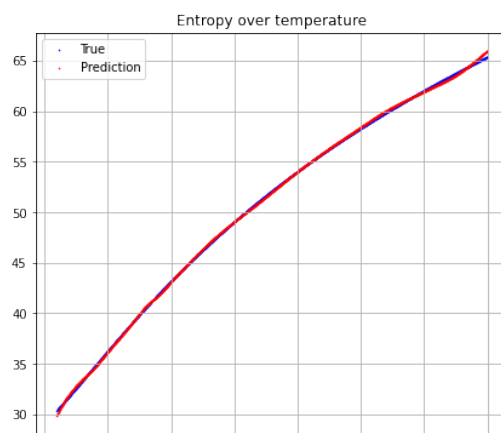
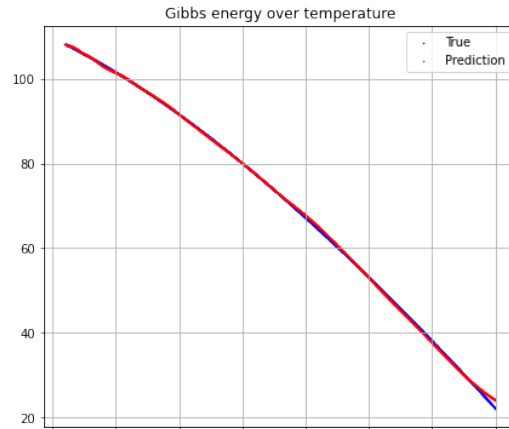
7000 : 0.32193057239055634

lr: [2.8587842838588265e-18]

3.921134131295341e-06

28.956972950159027 0.0001135441749738645 0.32179458141326905







7010 : 0.3217638283967972  
lr: [2.719018693194467e-18]  
-3.071463837915537e-07  
-378.15227409706773 0.00011614810351146679 0.3217880457639694

7020 : 0.32183878123760223  
lr: [2.5860862240230625e-18]  
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-141.91349310875324 0.00012735527333067716 0.3217953053116798

7030 : 0.3218105137348175  
lr: [2.4596528059263097e-18]  
-1.437201791880082e-06  
-93.75594122336217 0.00013474620672561976 0.3217944970726967

7040 : 0.32191863656044006  
lr: [2.339400701145074e-18]  
4.4338557184958943e-07  
295.0065338372244 0.000130801640704783 0.3217875871062279

7050 : 0.32160384953022003  
lr: [2.225027706077809e-18]  
-5.013784583734006e-06  
-25.287302026933325 0.000126785085066864 0.32179247856140136

7060 : 0.32171086966991425  
lr: [2.1162463918176223e-18]  
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155.9269856240259 0.00012608506690917114 0.32179701447486875

7070 : 0.3218660205602646  
lr: [2.0127833818193774e-18]  
-3.0331465662742146e-06  
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7080 : 0.32173971831798553  
lr: [1.9143786648815655e-18]  
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7090 : 0.3217507004737854  
lr: [1.820784941716396e-18]  
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-157.25802625161438 0.00011310140456626245 0.3218042656779289

```

7100 : 0.32180002331733704
lr: [1.7317670034659939e-18]
-2.723263234508281e-06
-42.13999629116963 0.00011475830260205756 0.32180752903223037

7110 : 0.3217164874076843
lr: [1.6471011406028601e-18]
-3.024327511690101e-06
-40.176290377812236 0.00012150626030726783 0.3218039524555206

7120 : 0.3219124674797058
lr: [1.5665745807291078e-18]
6.103089877537318e-06
20.57617939005694 0.0001255782721538485 0.3217974004149437

7130 : 0.3217650502920151
lr: [1.4899849538616237e-18]
-4.352355489925462e-06
-27.459684138437513 0.00011951430701154765 0.3217868447303772

7140 : 0.32188841700553894
lr: [1.4171397838593662e-18]
-1.3706027245034978e-06
-81.71236434370503 0.00011199518919510458 0.32179473310709

7150 : 0.3218846917152405
lr: [1.3478560047147174e-18]
1.0102379078767738e-06
106.53408786601665 0.00010762477404332505 0.32178853660821916

7160 : 0.32165881991386414
lr: [1.281959500493289e-18]
-4.9012656114539324e-06
-19.824393697694042 9.716461909843187e-05 0.3217910215258598

7170 : 0.3219175189733505
lr: [1.2192846677660077e-18]
3.771210203365404e-06
24.98420141994406 9.422067531782945e-05 0.32180108070373536

```

```

-----
KeyboardInterrupt                                Traceback (most recent call last)
<ipython-input-217-dbdce5ac5a0c> in <module>
----> 1 losses, best_net = train(net, dataloader, optimizer=optimizer,
    ↪ scheduler=scheduler, loss_func=loss_func, nr_epochs=nr_epochs)

```

```

<ipython-input-213-2efb855f2a93> in train(net, dataloader, optimizer, scheduler)
↳ loss_func, nr_epochs)
    33     for i in range(nr_epochs):
    34         #print('-----\nEpoch %i:\n' % i)
--> 35         loss = epoch(net, dataloader, loss_func, optimizer, scheduler)
    36         losses.append(loss)
    37

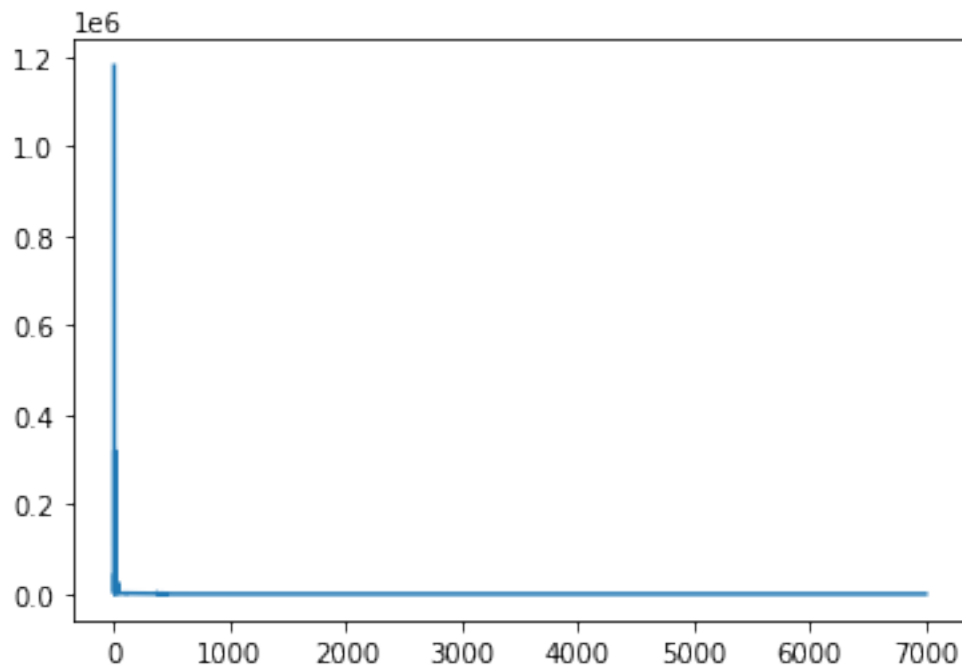
<ipython-input-213-2efb855f2a93> in epoch(net, dataloader, loss_func, optimizer
↳ scheduler)
    14         # Backward pass
    15         net.zero_grad()
--> 16         loss.backward()
    17         optimizer.step()
    18         epoch_losses[i] = loss

~\anaconda3\envs\5_Programmcodes\lib\site-packages\torch\_tensor.py in
↳ backward(self, gradient, retain_graph, create_graph, inputs)
    305             create_graph=create_graph,
    306             inputs=inputs)
--> 307         torch.autograd.backward(self, gradient, retain_graph,
↳ create_graph, inputs=inputs)
    308
    309     def register_hook(self, hook):

~\anaconda3\envs\5_Programmcodes\lib\site-packages\torch\autograd\_init__.py in
↳ backward(tensors, grad_tensors, retain_graph, create_graph, grad_variables,
↳ inputs)
    152         retain_graph = create_graph
    153
--> 154         Variable._execution_engine.run_backward(
    155             tensors, grad_tensors, retain_graph, create_graph, inputs,
    156             allow_unreachable=True, accumulate_grad=True) #
↳ allow_unreachable flag

```

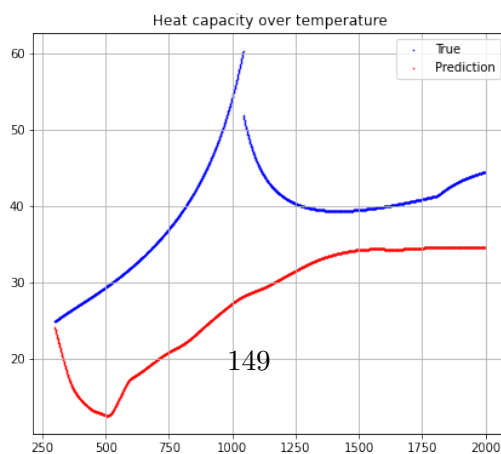
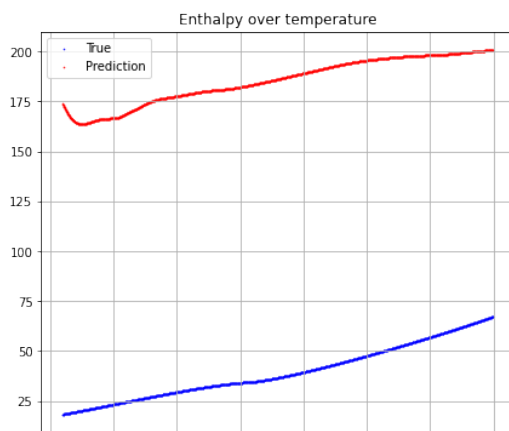
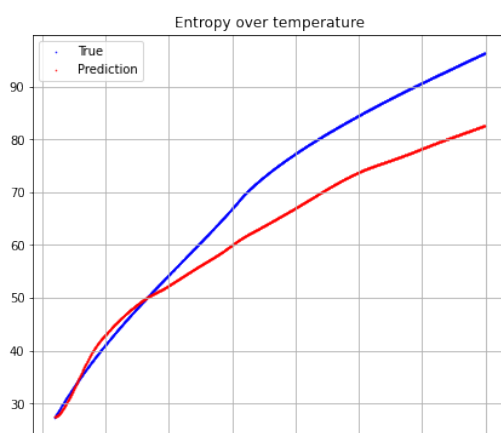
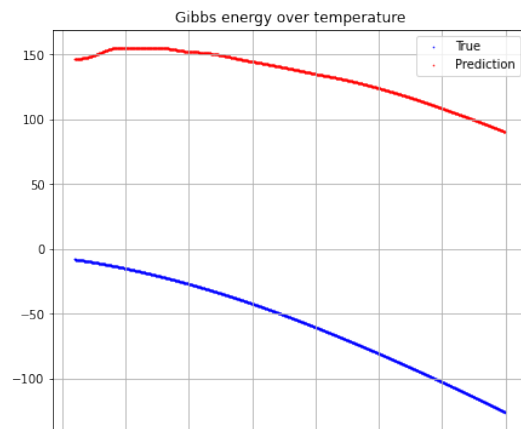
KeyboardInterrupt:



```
[ ]: plt.plot(losses[1400:])
```

```
[220]: #torch.save(net, 'C.pth')
```

```
[223]: ph = PlotHandler()  
  
ph.properties_temp_modified_new(net, ['Fe'], 'BCC_A2', start_temp=200,   
↪end_temp=2000)
```



[ ]: